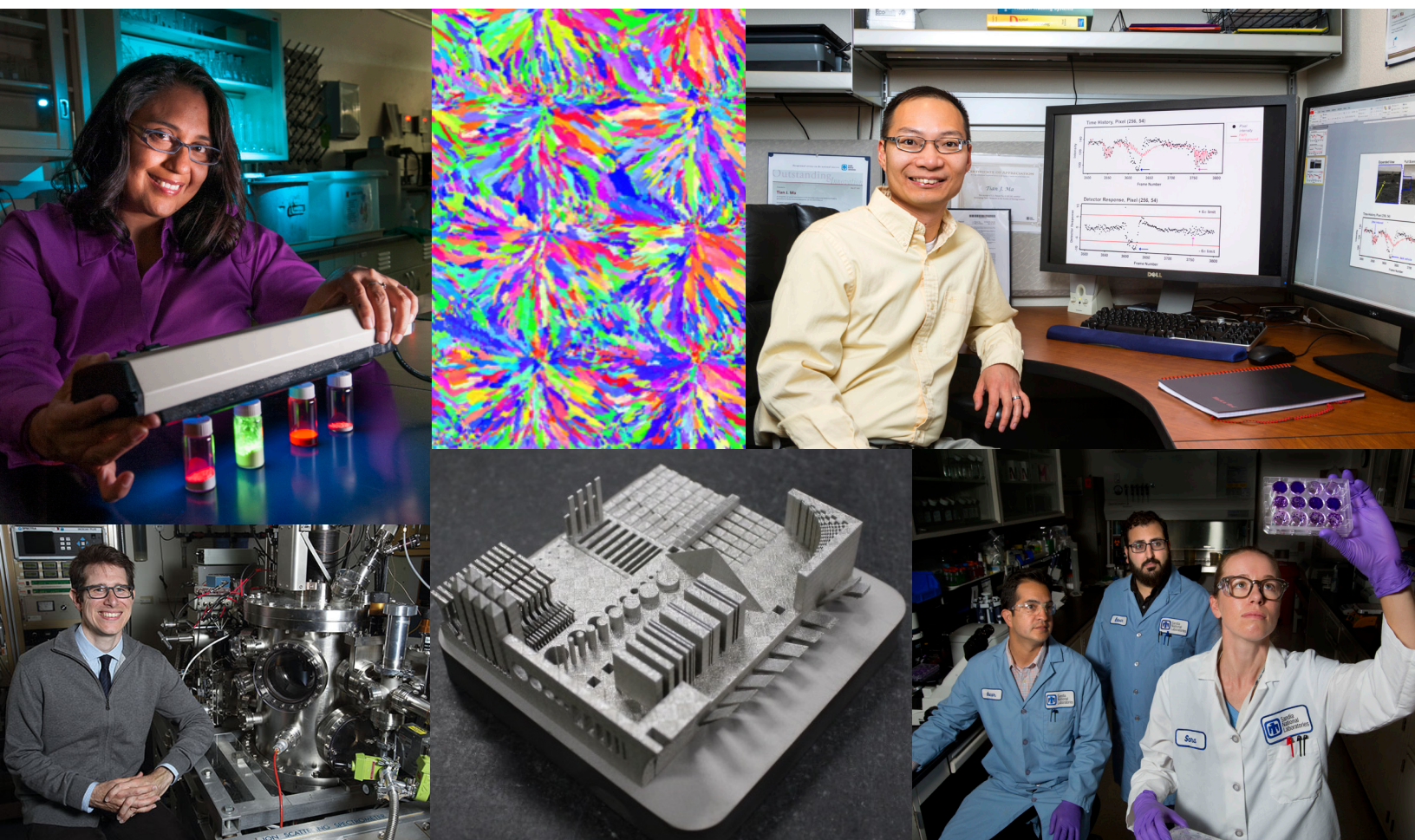


# Laboratory Directed Research and Development



## 2016 ANNUAL REPORT





# LABORATORY DIRECTED RESEARCH AND DEVELOPMENT



INNOVATION FOR OUR NATION

## FROM THE CHIEF TECHNOLOGY OFFICER



Over the past quarter century, Sandia's LDRD program has initiated innovations that have contributed to national security, ranging from ensuring the safety, security and reliability of the US nuclear stockpile to securing a sustainable energy future. In addition to enabling Sandia to create and sustain an environment of creativity and innovation, the LDRD program is significant because it expands Sandia's science and technology capabilities and contributes to our long-term vitality, enables Sandia to recruit and retain highly talented scientists and engineers, and has led to an impressive array of technological advances, awards, patents, and publications.

Each year, researchers across Sandia submit proposals for creative, forward-looking R&D projects that have the potential to greatly benefit our national security mission. NNSA guidance—as well as Sandia's internal LDRD processes—provides the framework for review and selection of Sandia's LDRD portfolio. Evaluation criteria include: alignment with Sandia strategy and potential national security impact; technical merit and feasibility; and leading edge, high risk R&D character. In a highly competitive FY2016 process, 689 short idea proposals were submitted. Of those, 187 were invited to submit full proposals, of which 111 were funded. When added to ongoing projects and late-start projects (which are also reviewed), 366 projects were active in FY 2016.

In this report, you will find descriptions of each of our active projects, as well as more information on Sandia's LDRD program. LDRD provides the knowledge that drives our future and continues to lead to many new scientific and technological breakthroughs that exemplify Sandia's commitment to exceptional service in the national interest.

**Rob Leland**

Chief Technology Officer  
Vice President, Science and Technology



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## ON THE COVER, LDRD IN THE NEWS IN 2016

Bernie Hernandez-Sanchez is the first woman at Sandia National Laboratories to win the 2016 Hispanic Engineer National Achievement Awards Conference Award for outstanding technical achievement. (Grand Challenges, Project 190245, 2016)

Electron Backscatter Diffraction map of advanced manufactured stainless steel. (Materials, Project 178667, 2016)

Robert Kolasinski received an Early Career Research Program award from the Department of Energy's Office of Science to support his work on how intense fusion plasmas interact with the interior surfaces of fusion reactors. (Grand Challenges, Project 173104, 2016)



Tian Ma was named the 2016 Most Promising Asian American Engineer, recognized for his achievements in developing new tracking algorithms for remote-sensing systems. (DS&A, Project 165555, 2015)

Oscar Negrete, Edwin Saada and Sara Bird check out a CRISPR library preparation. (Bioscience Project 180811, 2016)

Sandia Artifact printed in stainless steel alloy 17-4PH using a commercial vendor (Fineline) with a ConceptLaser Mlab Printer (Grand Challenges, Project 191144, 2016)



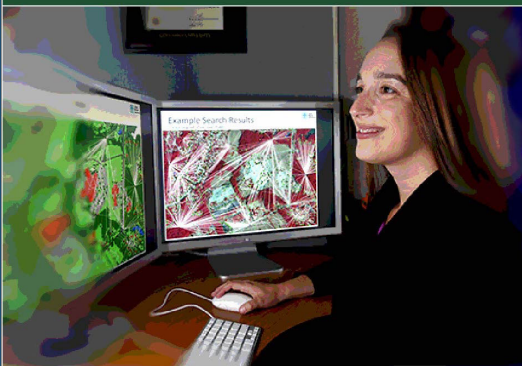
## A SNAPSHOT OF SANDIA'S LDRD PROGRAM

Sandia National Laboratories is charged with working on tough technical problems on behalf of the nation. Sandia's LDRD program is an essential element of the Laboratories' purpose to provide "exceptional service in the national interest."

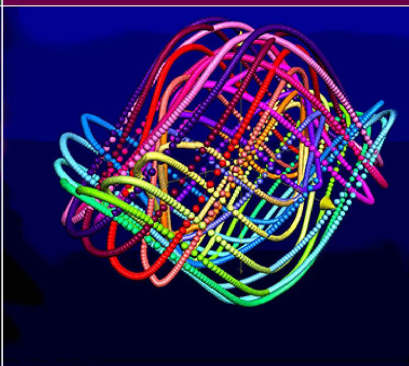
As Sandia's sole discretionary R&D program, LDRD funds foundational, leading-edge R&D that nurtures and enhances core science and engineering capabilities, supports national security missions, and leads to the creation of new capabilities.

## ENDURING LDRD PROGRAM GOALS

Enable our national security missions, now and in the future



Advance the frontiers of science and technology



Attract and retain a world-class research community



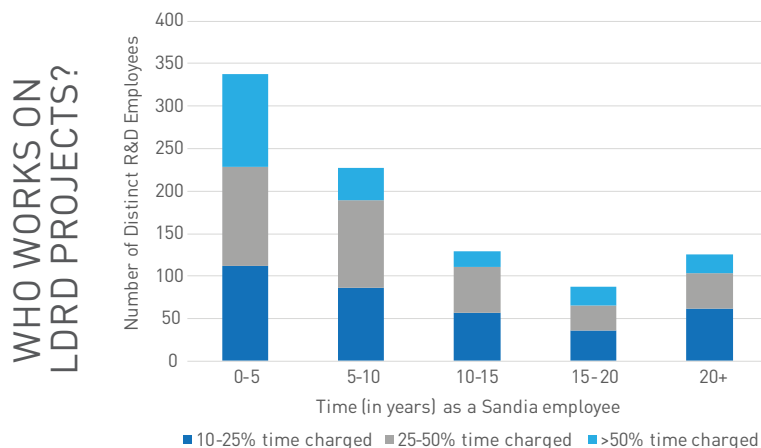
## FY 2016 LDRD PROGRAM STATISTICS

**\$155**  
[dollars, million]  
TOTAL LDRD  
PROGRAM COST

**\$300**  
[dollars, K]  
MEDIAN  
PROJECT SIZE

**366**  
[projects]  
TOTAL LDRD  
PROJECTS

**173**  
NEW IN  
FY 2016



**501** **44%**  
of all Sandia  
LDRD-SUPPORTED POSTDOCS  
[FY 2012 - 2016]

**87** LDRD-SUPPORTED  
POSTDOC-TO-STAFF  
CONVERSIONS  
[FY 2012 - 2016] **58%** of all Sandia

**31%**  
of all Sandia  
REFEREED  
PUBLICATIONS  
[CY 2011 - 2015]  
**1340 due to LDRD**

**47%**  
of all Sandia  
TECHNICAL  
ADVANCES  
[FY 2012 - 2016]  
**793 due to LDRD**

**52%**  
of all Sandia  
PATENTS  
ISSUED  
[FY 2012 - 2016]  
**286 due to LDRD**

**26%**  
of all Sandia  
SOFTWARE  
COPYRIGHTS  
[FY 2012 - 2016]  
**91 due to LDRD**

**81%**  
of all Sandia  
R&D 100  
AWARDS  
[CY 2012 - 2016]  
**16 due to LDRD**





## PROGRAM STRUCTURE

Sandia's research strategy arises from lab strategy: LDRD investments are based on a strategic and balanced portfolio of funding targets for major elements, known as Program Areas, which are further broken down into Investment Areas (IA). Each IA is focused on discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure and the allocation of funds to the associated IAs are designed to align LDRD investments with Sandia strategy and future mission needs.

LDRD investments provide cutting-edge foundational support for all of Sandia's strategic national security missions (Research Foundations), create and nurture the ability to provide innovative solutions for NNSA, DOE, and other Federal agencies (Mission Foundations), and address major research challenges to develop bold solutions to important national security challenges (Grand Challenges). The Corporate Investments Program Area supports strategic collaborations; special Lab fellowships; and Exploratory Express, an agile mechanism to test and mature novel R&D ideas.

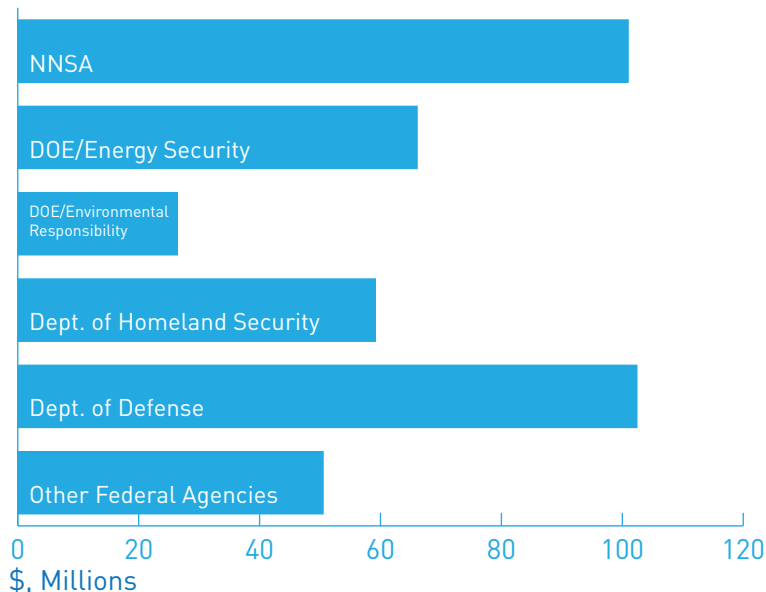
	Investment Area	Mission Impact and/or Laboratory Capability
RESEARCH FOUNDATIONS	Bioscience	Analyze, understand, and control the functions of biological systems in order to reduce global chemical and biological dangers and secure a sustainable energy future.
	Computing and Information Sciences	Advance the state of the art in computer and computational science and engineering, and information and data science relevant to national security.
	Engineering Sciences	Integrate theory, computational simulation, and experimental discovery and validation to understand and predict the behavior of complex physical phenomena and systems.
	Geoscience	Perform world-class R&D focused on the properties, structure, phenomena and processes associated with the earth's geosphere, hydrosphere, and atmosphere.
	Materials Science	Nurture foundational materials capabilities by developing methodologies to enable new understanding—or create enhanced understanding—of materials that are critical to our national security missions.
	Nanodevices and Microsystems	Perform creative, leading edge, and high-impact R&D to discover new phenomena at the nanoscale and microscale; and create or prove new concepts, devices, components, subsystems, and systems.
	Radiation Effects and High Energy Density Sciences	Advance the state of the art in radiation effects sciences, dynamic material properties, high energy density science, inertial confinement fusion, and pulsed power technology to enable stockpile stewardship and national security missions.
	New Ideas	Support pioneering research that may lead to game-changing breakthroughs in science and technology that could eventually impact national security.
MISSION FOUNDATIONS	Defense Systems and Assessments	Develop innovative systems, sensors, and advanced science and technology solutions to detect, deter, track, defeat, and defend against threats to our national security.
	Energy and Climate	Develop and create capabilities to contribute to the nation's energy security and resilience, economic viability, and environmental sustainability.
	International, Homeland, and Nuclear Security*	Support innovative science and technology that enhances our abilities to provide effective advice, analyses, technologies, and enterprise-level solutions to manage risks from the world's most dangerous events.
	*name changed to Global Security in FY2017	
	Nuclear Weapons	Nurture a creative and vibrant science, technology, and engineering base to support a deep scientific understanding of current and future NW products.
	Grand Challenges	Address bold science, technology, and engineering challenges requiring large multi-disciplinary teams to provide breakthrough solutions to critical national security challenges.
	Exploratory Express	Answer key research questions, within a relatively short timeframe, in an area of current or future strategic importance to Sandia. (Corporate Investments PA)



## MISSION-ENABLING RESEARCH

The LDRD program invests in research to enable mission success. As a multidisciplinary laboratory, Sandia brings researchers from all areas of science and engineering. By working together on LDRD projects, researchers develop leading edge solutions to both current and future challenges. From building foundational science capabilities to applied research to technology development, each LDRD project addresses one or more of the following: DOE/NNSA's missions, as well as the national security missions of the Department of Homeland Security, the Department of Defense, and Other Federal Agencies.

*\*Note that the dollar amounts at right are greater than the FY2016 program cost, since many projects are expected to benefit more than one mission and are therefore counted more than once.*



### Experiments and Computational Theory for Electrical Breakdown in Critical Components

PI: Fred Zutavern | Project 173097 | Engineering Science  
Anticipated to benefit missions of: NNSA, DOE



*Open shutter photograph of surface flashover near the high dielectric material used in lightning arrestor connectors. The event was triggered with a fine wire near the top of the dielectric stack. Photo credit: Zachariah Wallace.*

The phenomenon of electrical breakdown (EB) is a key issue for many electrical components, either the need to control it or prevent it entirely. For example, lightning arresters are designed to protect electrical systems by breaking down when struck by lightning. Predicting the performance and characteristics of these devices in extreme environments for stockpile and other critical applications is a key national security issue. For over a century, component designers have used the breakdown strength of bulk materials as a guide in many different environments, conditions, and configurations (that may have not been applicable or appropriate). Science-based modeling of EB has had limited success in predicting many important observed characteristics.

The goal of our work was to develop and apply unique experimental diagnostics, such as ultra-short pulse laser terahertz (THz) imaging of electron distributions, to determine the relative roles of electrons and ions during EB, and go beyond optical imaging to supplement the advancement of computational models. Most notably, we achieved sub-picosecond jitter timing for two ultrashort pulsed lasers integrated with an electrical pulse charging system and a high frame rate camera, enabling us to generate 2 picosecond THz pulses and record images from THz-plasma interaction.

We acquired 100 femtosecond time-resolved images of the THz radiation with good signal to noise ratios. The capability we developed can time-resolve extremely fast repetitive or single shot phenomena, such as those that occur during the initiation of electrical breakdown. Although we did not reach the goal of imaging electrical breakdown during this three-year project, the experimental technique developed and knowledge gained from the efforts will greatly enable new follow-on work that has derived from these efforts. No other plasma diagnostic provides this information, which is critical to modeling the initiation of electrical breakdown. We anticipate this LDRD-developed capability will improve models of the probability of electrical breakdown in components and complicated electronic systems.

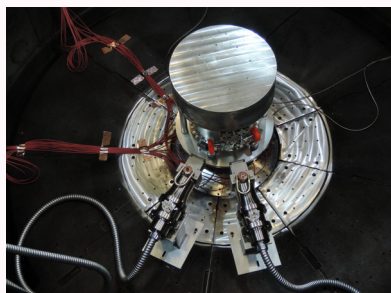




## MISSION-ENABLING RESEARCH

### FEATURE: NEW CAPABILITIES FOR RADIATION EFFECTS TESTING

Non nuclear components of nuclear weapons must be able to operate as intended in the hostile environments they may encounter during the stockpile-to-target sequence, specifically high neutron, x-ray, gamma ray, and electromagnetic pulse environments. Some of these environments can be physically simulated with high fidelity, but others can only be approximated or not physically simulated at all today.



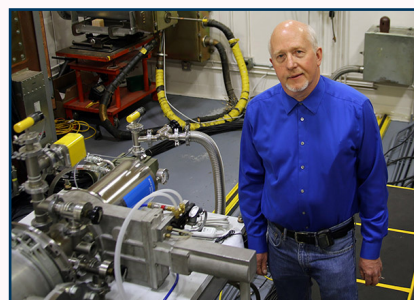
*Two fast neutron radiation-effects cassettes aim toward the center of the containment system for tritium within the Z vacuum chamber. The setup's gas transfer system is housed within the containment system.*

The **Hostile Environments Grand Challenge** (Project 173104) developed new x-ray and neutron test platforms with enhanced capabilities for nuclear weapons (NW)-relevant radiation effects science testing. The platforms opened new avenues for survivability testing, enabling the exposure of NW-relevant devices to higher neutron fluences and higher photon energies and fluences than ever before. The platforms were designed to ensure survival of the test devices and coupling with advanced diagnostics that provide a high fidelity characterization of the temporal, spatial and energy-dependent radiation environment. The project also developed the capability to safely use tritium in fusion targets on the Z facility for the first time (inset photo). Experiments were conducted at trace tritium levels (0.1 percent), and established a future path toward 50-50 deuterium-tritium mixtures, with a potential increase of a factor of 60-90 in neutron yields.

Led by Principal Investigator **Patrick Griffin**, the Hostile Environments Grand Challenge team comprised forty individuals. In addition to the team award featured below, several individuals were honored with professional achievements in FY2016.



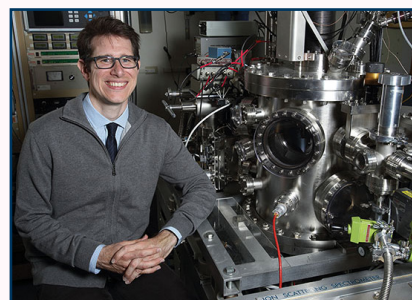
The team, which received an **NNSA Defense Program Award of Excellence**, successfully worked to push the frontiers in hostile environments research, accomplishing several remarkable feats, one of which enables the first use of tritium on the Z facility. Through their notable dedication, they have made truly pioneering improvements to the hostile environments research capabilities of Z whose value will have impact in years to come. This team has members in both New Mexico and California.



**Mark Savage**  
**William Dunbar Award, IEEE**  
For "continuing contributions to high voltage research, development, or testing technology and for transferring that technology to the engineering and scientific community."



**Christine Coverdale**  
**IEEE Plasma Science and Applications Award**  
For "outstanding contributions to the field of plasma science through research, teaching, and professional service to the scientific community."



**Robert Kolasinski**  
**Early Career Award, DOE**  
Robert's winning submission, "Characterizing the Dynamic Response of Surfaces to Plasma Exposure," was selected by the Office of Fusion Energy Sciences, which supports a broad range of plasma physics research activities.

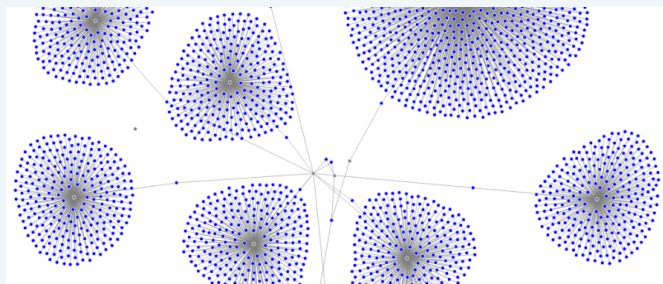


## MISSION-ENABLING RESEARCH

### Automated Discovery in Cyber Modeling and Simulation

PI: David Fritz | Project 180889 | Global Security  
Anticipated to benefit missions of: NNSA, DHS, DoD, OFAs

Our nation's critical infrastructures depend on distributed information systems, which must be resilient against malicious attempts to disrupt their operation. Security mechanisms must be deployed and continuously assessed to prevent adversaries from disrupting critical infrastructure. These information



*Support for large-scale, automatically generated models for emulalytics allows for novel test and evaluation and training environments.*

systems employ a broad range of technologies, enterprise architectures, cloud-based data centers, and emergency response wireless architectures. With the extensive reliance of critical infrastructure on secure information systems, new techniques and mechanisms to assess security must be created.

Efforts to extend state-of-the-art security modeling via emulation are hindered by our current ability to model meaningful emulations of real-world networks. To date, emulation research has focused on the means and mechanisms of emulation with little emphasis on fidelity or representative behavior of experiments. Our research identifies and attempts to resolve a critical gap in Sandia's existing cyber emulation and analysis environment (Emulalytics™)—the automated and efficient specification and generation of emulalytics models. This technology is intended to be leveraged by security researchers to build authentic and high-fidelity models of key networks in critical infrastructure domains. By leveraging high quality models, researchers will be able to better assess the security posture of target networks, and conduct any number of “what-if” scenarios. We created tools, that when integrated with Sandia's Emulalytics™ platform, can ingest real sensor data and output a detailed description of the network as visible from that sensor data. This capability is the first of its kind to support automated discovery and creation of arbitrary networks.

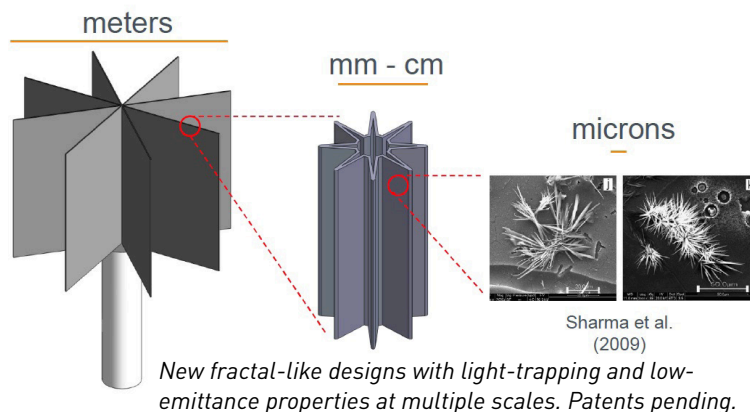
### Fractal-Like Materials Design with Optimized Radiative Properties for High-Efficiency Solar Energy Conversion

PI: Clifford Ho | Project 173092 | Energy and Climate  
Anticipated to benefit missions of: DOE

High temperature solar receivers and radiative heat collection components are used in renewable energy systems, space and satellite applications, and military operations to collect heat by maximizing solar absorption while minimizing thermal losses. However, at high temperatures (receivers can reach 600+°C), the radiative losses are significant.

While previous studies have tried to improve the efficiency of these receivers at high temperatures by increasing solar absorptivity and reducing thermal emissivity of surface coatings, very little research has investigated the optimization of features and radiative properties of receivers and other components at multiple length scales.

We designed and tested novel fractal-like structures and designs at multiple scales to maximize solar absorption while minimizing heat loss. The fractal-like geometries and features are introduced at both macro (meters) and meso (millimeters to centimeters) scales. We developed coupled optical/fluid/thermal models to evaluate the performance of these designs relative to conventional designs, which showed that fractal-like structures and geometries can increase the effective solar absorptance by 5–20% and the thermal efficiency by several percentage points at both the meso and macro scales, depending on factors such as intrinsic absorptance. We also fabricated meso-scale prototypes using additive manufacturing techniques, including a macro-scale bladed receiver fabricated with Inconel 625 tubes. We performed on-sun tests at Sandia's National Solar Thermal Test facility, which demonstrated enhanced solar absorptance and thermal efficiency of the new designs. These fractal-like designs will enable greater solar absorptance and thermal efficiencies for emerging solar-driven high-temperature power cycles of interest to DOE; there is also interest from international researchers and energy companies in the capability developed through this LDRD.







## MISSION-ENABLING RESEARCH

## PROJECT UPDATE



## BACKPLANE ANALYSIS SYSTEM BITES INFRASTRUCTURE BAD GUYS

Sandia's WeaselBoard helps critical infrastructure owners protect their systems against undisclosed software vulnerabilities. It is a small card that plugs into the backplane of an industrial controller to detect illicit traffic. WeaselBoard creates an assurance platform for responding to attacks as systems network together and scale up in the future.

Critical infrastructures, such as electrical power plants and oil refineries, rely on industrial controls to control essential processes. Such devices control billions of dollars worth of production, manufacturing, and utility equipment in the US. A cyberattack on these industrial control processes, many of which are unprotected, could have expensive and dangerous consequences. Most attacks focus on network communications and computer software, so industrial control systems, which are embedded at the hardware or firmware level, are not often monitored for security compromise. WeaselBoard works by detecting changes in the controllers and its processes and forwarding inter-module traffic to an external analysis system that detects changes. The analysis workstation then extracts fields at each protocol layer. "WeaselBoard allows operators to detect compromises as they are in progress, because it alerts on the effects of the attack in progress, and not on signatures of previously catalogued attacks. This allows exploits to be detected, unlike systems using signature-based detection methods," PI John Mulder says of the LDRD-developed technology.

PLC Backplane Analyzer for Field Forensics and Intrusion Detection, DS&A, Project 158752, 2012-2013. In the image above, PI John Mulder puts the WeaselBoard through its paces on a test apparatus.

PI: John Shadid | Project 173026 | Computing and Information Systems  
Anticipated to benefit missions of: NNSA, DHS, and DoD

## Towards Rigorous Multiphysics Shock-Hydro Capabilities for Predictive Computational Analysis

Many critical science and weapons applications require predictive analysis of complex shock hydrodynamics with electromagnetics. The physical mechanisms include wave phenomena, material transport, diffusion, chemical reactions, and electromagnetics. The highly nonlinear multiple-time and length-scale response of these systems includes discontinuities formed from shocks, contact surfaces, and complex tabular equations-of-state. Current computational solution strategies use ad hoc mathematical combinations, which lack the stability, accuracy, and efficiency needed to resolve all the dynamic time scales of interest. They also lack the ability to perform integrated fast sensitivity analysis and uncertainty quantification (UQ).

To address this challenge, we have developed a unique, modern, mathematical/computational approach for multiphysics shock-hydro with integrated sensitivity and UQ analysis techniques for specific scientific quantities of interest (QoI) (e.g., localized measures of momentum and kinetic and magnetic energy). New computational algorithms and software allows for efficient higher-order integration of multiphysics and solution of both multiple time-scale systems and fluid motions. Adjoint methods enable fast and efficient determination of parameter sensitivities, and construction of UQ models for QoIs. The work is already impacting several nuclear weapons mod/sim applications, and is being incorporated into the open-source software package Trilinos, used by Sandia and DOE for multiphysics modeling. Additionally, the capability developed through this project also enhances research in radiation effects, dynamic materials, and high energy density laboratory physics efforts in Sandia's pulsed power research area.



## AT THE FOREFRONT OF SCIENCE AND ENGINEERING

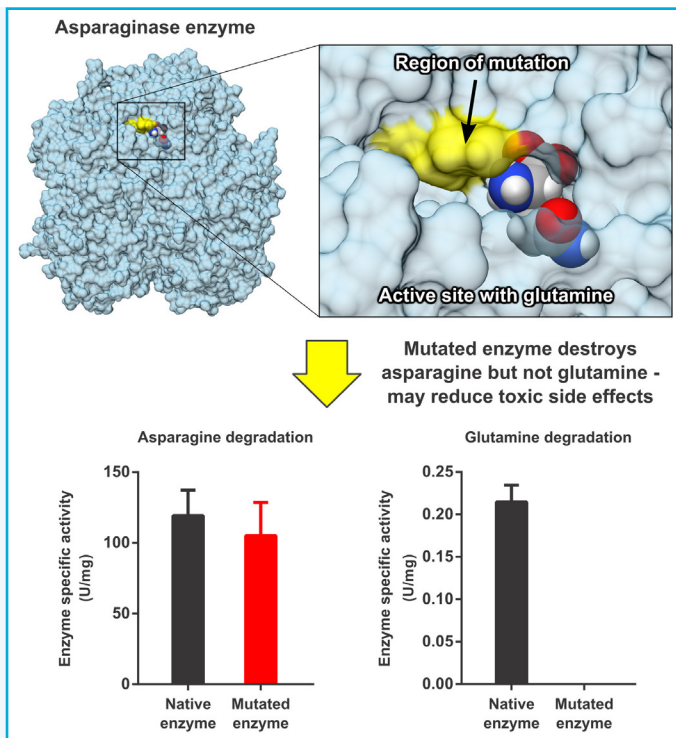
Sandia is a 21st century, broad spectrum national security laboratory, and LDRD research plays an essential role in maintaining the Labs' scientific vitality. As the nation's most diverse national security laboratory, Sandia is uniquely equipped to tackle groundbreaking interdisciplinary research challenges. Tackling these challenges allows the Lab to fulfill its responsibilities and core national security mission work, while simultaneously advancing related mission areas of value to our nation. In order to fulfill its national security mission, Sandia must remain at the forefront of multiple scientific areas.

### Probing Small-Molecule Degradation to Counter Enzyme Promiscuity

PI: Susan Rempe | Project 173142 | New Ideas  
Anticipated to benefit missions of: DHS, DoD, CDC

Enzymes that degrade specific small molecules could save lives by neutralizing threats from chemical agents in the blood or environment, but promiscuous interactions with other molecules typically limit their effectiveness by blocking the enzyme active site. An obvious solution is to re-engineer the enzyme to enhance catalytic fidelity, but lack of understanding about how enzymes discriminate between molecules remains a formidable challenge to this approach. Our recent work in collaboration with the University of Texas (UT) suggests a new approach and a model system for understanding enzyme specificity. Asparaginase enzymes catalyze degradation of asparagine—an amino acid that feeds some cancers—which forms the basis of a medical treatment. Competition by other abundant molecules interferes with asparagine decomposition, thus hindering enzyme efficacy. Asparaginase is advantageous as a model degradation enzyme because variants that demonstrate different binding affinities and catalytic rates can be compared.

Our preliminary work suggests that the mechanism of molecular specificity in asparaginase depends on a different set of chemical interactions than previously speculated. We have leveraged Sandia's strengths in molecular simulation and UT experimental expertise in asparaginase modification and functional assays to understand enzyme degradation of small molecules. Our simulations probe how local properties of the asparaginase active site determine molecular binding affinities and free energy barriers to degradation, and predict mutations (tested experimentally) to tune catalysis to favor a specific molecule. The project led to the development of a new strategy to re-engineer safer and more effective enzymes to break down small molecules. That strategy was demonstrated for a leukemia drug, with potential therapeutic applications to leukemia and other cancer cells. The strategy is broadly applicable to improve enzymes that break down chemical warfare agents for therapeutic and decontamination applications.



*A simulation by researchers at Sandia and the University of Maryland demonstrates that a mutated enzyme will degrade asparagine—food for some cancers—but leave glutamine, necessary for all proteins, untouched. (Graphic by Juan Vanegas)*



Want to learn more about  
about LDRD research  
happening at Sandia?

Check out the Sandia Research Magazine

[http://www.sandia.gov/news/publications/research\\_magazine/](http://www.sandia.gov/news/publications/research_magazine/)



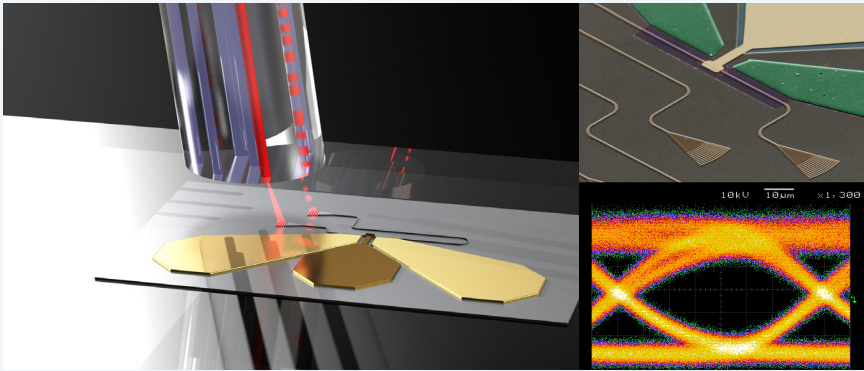




## AT THE FOREFRONT OF SCIENCE AND ENGINEERING

PI: Gordon Keeler | Project 192700 | Exploratory Express  
Anticipated to benefit missions of: NNSA

### Probing Charge Layers in Conducting Oxides for Next-Generation Plasmonics



First demonstration of a high-speed nanophotonic modulator based on carrier density modulation in transparent conducting oxides. Left: Integrated modulator. Top Right: Colorized scanning electron microscope image of fabricated device. Bottom Right: 2.5Gbps eye diagram.

Plasmonic approaches to optical signaling promise order-of-magnitude size reductions beyond conventional photonic limits, and could enable revolutionary improvements in power dissipation, integration density, and functionality for computing, sensing, and communications. Recent reports of compelling plasmonic modulators suggest that they may be the first practical, high-speed nanoplasmonic devices. These modulators operate by strongly altering the carrier density of conducting oxide layers. Such films are not traditionally used in high-speed photonics, and materials

limitations (including leakage current filaments through dielectric layers or charge trapping at grain boundaries and interfaces) may explain why experimental work to date has failed to demonstrate even moderately high-speed switching. The goal of this project was to study the dynamics of the essential charge layer in high-quality conducting oxide films to assess the feasibility of efficient, ultrafast plasmonic modulators.

This project explored the key physics and practical limitations of controlling charge carrier density in thin conducting oxide layers, with the goal of enabling next-generation plasmonic devices with high potential impact. Specifically, this work looked to demonstrate that sufficiently large carrier densities can be obtained in the conducting oxide films, that dielectric leakage paths are nondominant sources of carrier density, and that electron accumulation layers can be created and removed at high speeds. These topics further our scientific understanding of materials and interface limitations for oxide-based plasmonic devices, and highlight a path to compelling practical devices with significant potential impact on DOE-relevant mission areas, including compact, ultrafast, low-power optical communications modulators for next-generation computing systems.

### PROJECT UPDATE



#### THOR'S HAMMER DESIGNED TO CRUSH MATERIALS AT ONE MILLION ATMOSPHERES

Sandia's newest accelerator concept, called Thor, is focused on generating high pressures to study materials under extreme conditions. While it will not be able to generate as much pressure as Sandia's Z machine, the world's largest and most powerful pulsed power accelerator, when completed, Thor will be smaller and up to 40 times more efficient due to design improvements that use hundreds of small capacitors instead of Z's few large ones. These capacitors discharge current in a 100-nanosecond pulse immediately, obviating energy losses inevitable when compressing a long pulse. The new architecture also allows finer control of the pulse sent to probe materials, allowing different types of materials science experiments than are possible on Z. Thor's theoretical design was supported by Sandia's LDRD program, with later engineering details and hardware supported by the National Nuclear Security Administration's Science Campaign.

Investigate Emerging Material Technologies for the Development of Next Generation Magnetic Core Inductors for LTD Pulsed Power Drivers, REHEDS, Project 158861, 2012-2014. In the image at left, Eric Breden installs a transmission cable on the silver disk that is the new pulsed power machine's central powerflow assembly.



## A WORLD-CLASS RESEARCH COMMUNITY

Sandia's specialized missions require highly motivated, qualified staff with deep expertise, committed to advancing the frontiers of science and engineering through continual growth and development. The LDRD program supports some of Sandia's most accomplished scientists and engineers, as well as many promising early career researchers. Some selected accomplishments are highlighted below.

Jon Ihlfeld

**Ferroelectrics Young Investigator Award**  
**IEEE Ultrasonics Ferroelectrics and Frequency Control Society**

Jon's award is a nod for significantly advancing the processing and integration science of thin film ferroelectrics for practical applications.

Conrad James



**Black Engineer of the Year Award**

Conrad uses his background in neural engineering to investigate microelectronic devices for brain-inspired computing. Conrad is currently a PI on a Grand Challenge LDRD project.

Cindy Phillips

**Distinguished Scientist**  
**Association of Computing Machinery**

Cindy, a senior scientist in Sandia's Center for Computing Research, conducts research in combinatorial optimization, algorithm design and analysis and parallel computation.



**Bernie Sanchez**  
**Hispanic Engineer National Achievement Awards Conference award**

Bernie's technical achievements focus on the morphology, structure and properties of nanomaterials for real-world applications that range from renewable energy to homeland security.

Phillip Reu

**Brewer Award, Outstanding Experimentalist**  
**Society of Experimental Mechanics**

Phillip develops new techniques for large-scale and high-rate full-field measurements for application to explosively driven events.

Shanalyn Kemme

**SPIE Senior Member**  
**International Society for Optical Engineering**

Shannon's achievements in design and development of micro-optical systems and diffractive optics contributed to this recognition.



Vince Urias

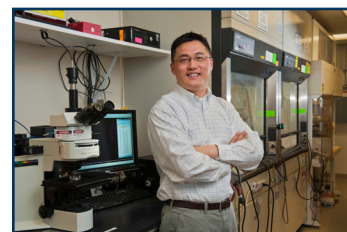
**Hispanic Engineer National Achievement Awards Conference award**

Vince was named a luminary honoree for his success with community outreach and Sandia's cyberdefense programs.

Hongyou Fan

**Fellow of the Materials Research Society**

Hongyou's nanotechnology work was cited for "pioneering contributions to the development of novel synthesis methods and self-assembly processes to fabricate multifunctional nanomaterials for nanoelectronic and nanophotonic applications and service to the materials community."



David Osborn

**Presidential Early Career Award for Scientists and Engineers**

David was honored "for innovative research in multiplexed methods for interrogating chemical kinetics and measurements of the physical chemistry of previously elusive reaction intermediates."



Ali Pinar

**Distinguished Scientist**  
**Association of Computing Machinery**

Ali's focus is on modeling and analysis of graphs and using sampling and streaming algorithms for massive data sets, research that has garnered many best paper awards.



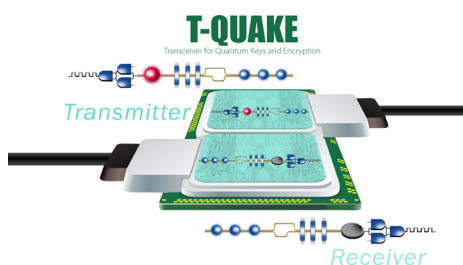
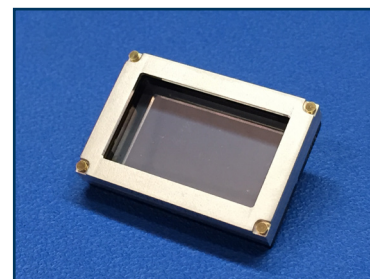


## A WORLD CLASS RESEARCH COMMUNITY

Competing in an international pool of universities, corporations, and government labs, Sandia inventions and co-inventions captured six R&D 100 Awards this year. R&D Magazine presents the awards each year to researchers who its editors and independent judging panels determine have developed the year's 100 most outstanding advances in applied technologies. Four of the winning Sandia technologies had their roots in the LDRD program. In fact, over the past five years, about 80 percent of Sandia's R&D 100 Award winning technologies have involved some investment by LDRD.

### UXI (Ultra-Fast X-Ray Imager)

The fastest multiframe digital x-ray camera in the world that takes images with an exposure time of only 1.5 nanoseconds—25 times faster than the best digital cameras. It helps researchers capture plasma images more rapidly, and has already been used successfully in hundreds of experiments at Sandia's Z-Beamlet laser facility and at Lawrence Livermore National Laboratory's National Ignition Facility. PI: John Porter

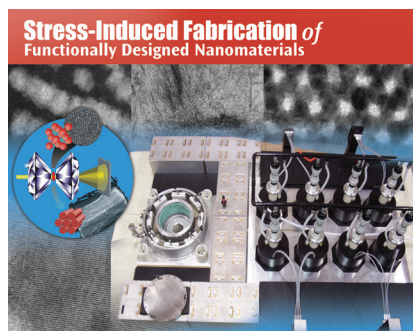


### T-QUAKE (Transceiver for Quantum Keys and Encryption)

Miniaturizes all of the components necessary to securely encode, transmit, receive, and decode quantum photonic signals onto a single microchip, in effect creating an ultra-secure cryptographic network node for any secure communication or network application. PI: Ryan Camacho

### Pyomo v4.1

An extensible software platform for developing optimization-based analytics to support complex decision making in real-world applications. Optimization—finding a solution that minimizes (or maximizes) a function over a set of possible alternatives—is widely used in business, science, and engineering to minimize costs, identify worst-case scenarios, and analyze trade-offs. Optimization is used to schedule commercial aircraft and crews, manage supply chains for auto manufacturers, design sensor networks to protect water distribution systems, identify locations for military supply depots, and operate power grids worldwide. PI: William E. Hart



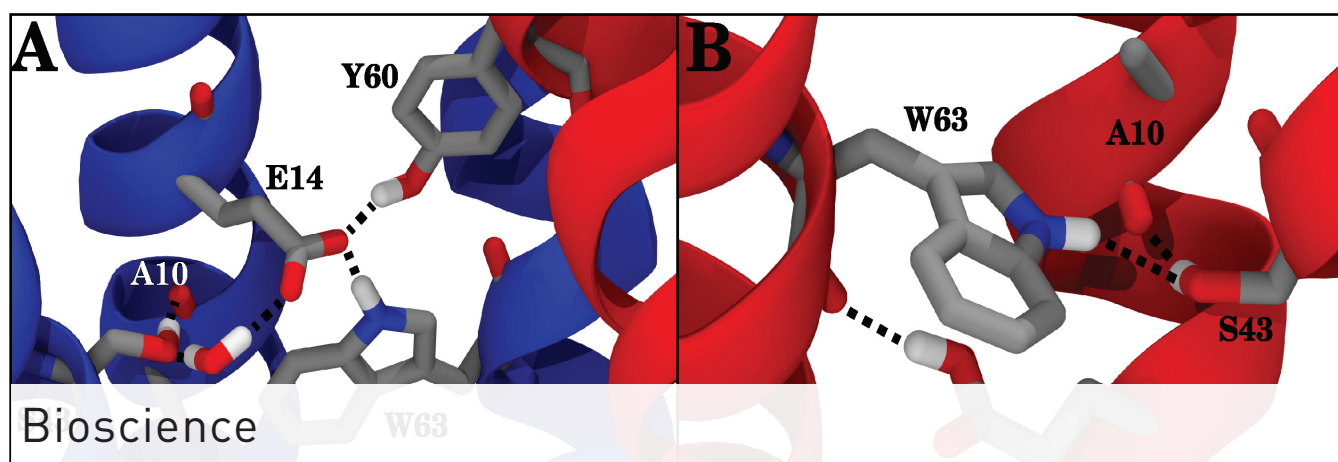
### Stress-Induced Fabrication of Functionally Designed Nanomaterials

Enables the production of new materials with better performance and structure control while reducing costs, improving manufacturability, and minimizing environmental and safety concerns. The technology represents a new paradigm for the production of functionally designed nanomaterials with more degrees of freedom than chemical methods. PI: Hongyou Fan

## Research Excellence in Service of the Nation

LDRD supports Sandia's mission by investing in leading-edge research that advances the frontiers of science and engineering critical to national security. The program is also instrumental in attracting and developing a world-class workforce of scientists and engineers, the people who make it possible for Sandia to achieve its mission and goals.

To learn more, visit [www.sandia.gov/ldrd](http://www.sandia.gov/ldrd).



The overarching goal of the Bioscience Investment Area is to develop new competencies in biological science to address two application areas in Sandia's broad national security mission—biodefense and emerging infectious disease, and biofuels. The research in biodefense includes developing better ways to detect, characterize, and contain harmful pathogens. The strategy integrates advanced technologies with an understanding of human health and immune response. The goal is to improve the response to disease outbreaks and to limit their spread. The research regarding the nation's reliance on fossil fuels focuses on developing efficient, economical biofuels that can replace or reduce current gasoline, diesel, and aviation fuel consumption. The research includes two sources of energy: lignocellulose, or dry plant matter, and algae. The aim is to find efficient and economical methods to convert lignocellulose into fuels and to understand the factors that govern algal pond stability and identify molecular mechanisms that can be used for lipid/fuel production.

*The figure above shows examples of hydrogen bonding (black dashed lines) during a simulation, and how the bond changes with the protonation of glutamate; the two panels illustrate different types of monomer interactions. Understanding these processes will provide insight into the transport of drug-like molecules across bacterial membranes in order to develop novel treatment approaches. (Project 180817, Coupling Chemical Energy with Protein Conformational Changes to Translocate Small Molecules Across Membranes)*

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## Analyzing and Understanding of Transporters to Control Lignin Transformation into Fuel

190958 | Year 1 of 3 | Principal Investigator: J. A. Timlin

### Project Purpose:

The production of drop-in transportation fuels is critical to meeting our nation's alternative energy goals. Lignocellulosic biomass, an abundant and renewable fuel source, is poised to meet that need. However, economic viability requires that the value of the lignin content surpass that obtained from its combustion. Although lignin breakdown and conversion occurs in natural microbial communities, we lack the necessary understanding to design an efficient industrial biological process to convert lignin to renewable fuels and chemicals. Lignin transporters are essential to this process; rapid transport of lignin breakdown products into and transport of product out of a conversion host will be required. Yet the transport mechanisms are poorly understood due to the chemical diversity of lignin breakdown products and the lack of a toolset for analyzing the uptake and metabolism of lignin within lignolytic microbes. This project harnesses several unique internal capabilities and leverages external collaborations with DOE facilities to characterize lignin transport in fungi and bacteria. We will develop new methodologies to analyze transport of lignin breakdown products into microbes and will provide a foundational understanding of the range of substrates, kinetics, and structural biology of lignin transporters. The research proposed here will be the first systematic study of lignin transporters. Knowledge gained from this project will enable increased lignin transport into and out of industrially-relevant microbes and therefore increased lignin conversion to fuels and chemicals.

This project will define basic scientific principles required to engineer solutions for lignin-based fuel production by targeting the biological valorization of lignin. We will utilize Sandia's core strengths in imaging, structural and computational biology, and lignin analytics.

## Bio-Emulative MOF-Based Lignin Degradation Catalysts

180812 | Year 2 of 3 | Principal Investigator: M. D. Allendorf

### Project Purpose:

Lignin is the most abundant source of renewable aromatics, with 200-300 Mtons/yr projected production by a US biofuels industry that would process ~1B tons of biomass to meet DOE goals. However, there are currently no efficient processes for extracting these aromatics and converting them to value-added chemicals and drop-in fuels. The technical and economic challenges are staggering, due to the quantities of material involved and lignin's recalcitrance to depolymerization. Conventional lignin degradation processes use aggressive reagents and are energy intensive (400-800 °C) and yield complex product mixtures. Milder reaction conditions and narrower product distributions could be achieved using lignin-degrading enzymes, but these are too fragile to be practical for large-scale biorefining. The objective of this project is to develop lignin valorization methods in which oxidative solubilization provides a feedstock for industrially robust catalysts based on metal-organic frameworks (MOFs). MOFs are nanoporous materials with exceptional synthetic versatility arising from a structure comprised of metal ions linked by rigid organic groups. Our strategy is to tailor selected MOFs for either reductive or oxidative lignin decomposition reactions. We are employing computational chemistry and in situ diagnostic probes to obtain structural and energetic knowledge of MOF catalysts.

This year we expanded our suite of MOF-based hydrogenolysis catalysts and optimized the pore size to maximize conversion of aryl-ethers to small molecules. We also demonstrated a new class of oxidation catalysts that cleave common carbon-oxygen bonds in lignin with >99% conversion and >90% selectivity. Finally, we showed that the products of our lignin pretreatment method, which employs an inexpensive homogeneous catalyst based on the Fenton reaction to control the molecular weight distribution of solubilized products, can be tuned from polyacids to aromatic lignin monomers simply by altering the solvent. These results confirm the original project hypothesis that MOFs provide a versatile platform for developing lignin valorization catalysts.





## Coupling Chemical Energy with Protein Conformational Changes to Translocate Small Molecules Across Membranes

180817 | Year 2 of 2 | Principal Investigator: S. Rempe

### Project Purpose:

All living cells rely on continuous exchange of diverse molecular species (e.g., nutrients, precursors, and reaction products) across cellular membranes for their normal function and survival. Membrane transporters are specialized molecular devices that provide the machinery for selective and efficient transport of materials across the membrane. The biological significance of membrane transporters cannot be overstated, given their central role in myriad key cellular processes and their subsequent targeting by a large number of pharmaceuticals. The significance of membrane transporters is also evident from a recent major focus shift of experimental structural biological studies toward characterizing structural states arising during the function of these proteins. Currently, our understanding of active membrane transport is limited. Experimental methods provide only snapshots of the energy-coupled transporter activity. Our goal is to obtain an understanding of the full mechanism. Specifically, we endeavor to understand how chemical energy in a cell couples with the mechanics of protein conformational changes to produce directional translocation of a specific substrate across cellular membranes. To achieve this understanding requires a dynamical description of structural transitions during the transport process and the free energy barriers along the transport pathway. We used molecular simulation to achieve those goals. Our specific target is to identify the molecular mechanism of drug export by a bacterial (*E. coli*) transport protein called EmrE.

## Deciphering Global Dynamics of Microbial Multidrug Resistance Regulation using Microfluidic Cross-linking Kinetic Analysis and Ultra High-throughput Sequencing ( $\mu$ CLK-seq)

192788 | Year 1 of 1 | Principal Investigator: K. Poorey

### Project Purpose:

The emergence of multi-drug resistant (MDR) bacteria translates to \$20 billion/year in excess healthcare in the US alone. Further, a lack of tools, assays, and reagents to study these emerging pathogens has made it difficult to devise treatments. If left unaddressed, MDR bacteria will pose an enormous threat to US national security by crippling both the economy and the health of the population. We proposed a study aimed towards understanding MDR bacteria's genetic and signaling responses to antibiotics, and the molecular mechanisms underlying the regulation and evolution of antibiotic resistance. The activation of the defenses in the presence of drugs and the transcription changes are quite difficult to measure from pre-existing assays. Hence, to understand MDR bacteria's resistance mechanism and to find the new biomarkers, we developed a new assay (cross-linking kinetic, CLK-Seq) that measures the genome-wide transcriptional regulation at a seconds time scale. We designed a novel microfluidic system to precisely and automatically stimulate, crosslink, and quench protein/DNA interactions in MDR bacteria as they respond to antibiotics. This microfluidic device was used in conjunction with ultra high-throughput sequencing to profile the MDR *Klebsiella pneumoniae* responses to antibiotics. The CLK system has enabled the collection of kinetic information on protein/DNA interactions that underlie mechanisms of MDR regulation by pushing the detection of protein/DNA interaction to a seconds time scale. Significant effort was used in computational analysis of MDR gene regulation and its correlation with the transcriptional response. A technical advance for the new device is under way and the work for the characterization of the mixing is also being presented at the October 2016 microTAS conference. We have developed a novel generic assay to characterize the dynamics of any organism without the use for antibodies and used it to characterize the MDR pathogen *K. pneumoniae* for the first time ever.



## Discovery of Anti-Viral Inhibitors Against the Chikungunya Virus nsP2 Protease Domain

186364 | Year 2 of 3 | Principal Investigator: B. N. Harmon

### Project Purpose:

Chikungunya virus (CHIKV) is an emerging mosquito-borne alphavirus that causes devastating arthritic disease. CHIKV has been responsible for major outbreaks in Africa and Asia leading to serious morbidity and mortality in humans. The first cases of CHIKV were reported in the Western Hemisphere in late 2013 and nearly one million suspected CHIKV infections have occurred in the Americas in the last year. The CHIKV mortality rate has been estimated to be 1:1000. The US National Institute of Allergy and Infectious Diseases lists CHIKV as a category C biodefense priority pathogen due to the ability to engineer this pathogen for mass dissemination and the current debilitating effects of the virus on infected warfighters. At present, there are no licensed vaccines or treatment options to combat CHIKV infection, and research in the development of therapeutics has been limited. To develop timely countermeasures against this biological threat, this project seeks to discover lead compounds for the treatment of CHIKV. Specifically, we will discover small molecule inhibitors of the viral nsP2 protease (nsP2pro) using advanced bioinformatics, cheminformatic, and experimental screening methods. Viral nsP2pro is a cysteine protease encoded as part of the viral nonstructural polyprotein, and is essential for polyprotein processing and viral reproduction. At the end of the project, our goal is to have in hand small molecule inhibitors that meet three criteria: 1) effective inhibition of nsP2pro proteolytic activity, demonstrated in vitro and cell-based assays; 2) low inhibition of human proteases and low cytotoxicity; and 3) robustness to resistance due to sequence mutations.

We seek to discover CHIKV therapeutics using our drug discovery pipeline that includes compound screening with novel fluorescence resonance energy transfer-based high-throughput assay, computer-aided modeling and structural activity relationship for down selection of candidate inhibitors, and validation of selected compounds using cell based assays to measure safety and efficacy against infection with CHIKV. Unique combined expertise in biodefense, modeling/simulation can accomplish these objectives.

## Engineering 'Green' Algae: Reducing Metabolic Waste for High Biomass Productivity

190962 | Year 1 of 3 | Principal Investigator: A. Ruffing

### Project Purpose:

The July 2014 Multi-Year Program Plan for the Bioenergy Technologies Office (BETO) sets forth a goal of demonstrating algal productivities greater than 5,000 gallons of biofuel intermediate per acre per year (gal/acre/yr) by 2025. Traditional efforts to improve algal productivities via bioprospecting and algal raceway design have led to current productivities of approximately 1,500 gal/acre/yr. To achieve BETO's productivity goal in the next ten years, new algal strain development methods, such as genetic modification, and subsequent reprogramming of the metabolism of algal production strains are necessary.

Natural algal metabolisms evolved under low oxygen conditions for the purpose of optimizing organism survival, resulting in algal strains that lose fixed carbon due to photorespiration and nighttime respiration (i.e., "dark loss") to enable reproduction. Photorespiration also leads to the wasteful generation of ammonia and subsequent energy consumption for refixation. We propose to develop tools for genome engineering of the industrially relevant alga, *Nannochloropsis gaditana*, and to utilize these new tools to reduce metabolic waste associated with photorespiration and dark respiration. If we are able to achieve the 30-50% increase in growth reported for plants expressing bacterial photorespiratory bypass pathways and also eliminate the 50-60% dark loss observed for *Nannochloropsis* growth in open ponds, the modified *Nannochloropsis* strain would be a significant step towards BETO's productivity goal, with calculated productivities ranging from 2,700 to 3,150 gal/acre/yr. Additionally, the genetic tools developed in this project would enable future strain development efforts for synthesis of various chemical and biofuel targets.





## Exploiting the Microbial Achilles Heel for New Broad Spectrum Anti-Microbials (NBSAMs)

190961 | Year 1 of 3 | Principal Investigator: S. Rempe

### Project Purpose:

Bacteria resist traditional antimicrobials, costing the US \$45B annually in drug-resistant infections and loss of life. Recent discovery of the first new class of antimicrobial molecule in 30 years (*Nature*, 2015) provides a potential game-changing opportunity. Gram-negative bacteria produce Teixobactin (TXB) to kill gram-positive bacteria. TXB binds primary lipid precursors needed to synthesize the protective bacterial cell wall, thus exposing a microbial Achilles heel. Binding disrupts cell wall synthesis or leads to uncontrollable release of cell-wall-degrading autolysins—both are lethal. TXB is a proven bacteriocide, active against several gram-positives (e.g., *Bacillus anthracis*) and with low susceptibility to triggering resistance. Though promising as a potential therapeutic, TXB is not ideal because of inconsistent effectiveness across bacterial strains. We hypothesize that variability arises due to target inaccessibility caused by differences in bacterial cell walls. Highly effective antimicrobials would still target the crucial Lipid II/III combo, but also reach those targets more readily. A range of TXB variants is needed to achieve broad spectrum activity. An understanding of the molecular interactions between TXB, its lipid targets and the cell wall could result in variants that achieve the desired functions. By using molecular simulation, quantitative binding assays, and state-of-the-art synthetic strategies to test mechanistic hypotheses, we may achieve a breakthrough in understanding and demonstrate TXB tunability for the first time. Success will result in the first molecular understanding of a new class of antimicrobial and the first variant(s) more effective in reaching the lipid targets, potentially leading to highly potent and broad-spectrum antimicrobials.

## In Vivo High Throughput Transcriptomics to Elucidate the Spatial and Temporal Dynamics of Host-Pathogen Interactions

173021 | Year 3 of 3 | Principal Investigator: R. Meagher

### Project Purpose:

Drug-resistant bacterial infections are a re-emerging health crisis, ranging from community-acquired Methicillin-resistant *Staphylococcus aureus* (MRSA) to hospital-acquired infections. Drug-resistant infections associated with injuries to warfighters and treatment in hospitals have been highly problematic. The purpose of this project is to develop and characterize a new technique for studying bacterial pathogenesis at the level of RNA transcription. The technique involves solution-phase hybridization with probes representing the entire bacterial genome, at high depth, followed by capture of the probes with bound transcripts, and preparation of next-generation sequencing libraries.

While the basic methodology was previously established, this project was looking specifically at improving the throughput of the technique to enable us to process samples more efficiently and to study larger, more complex problems in microbial pathogenesis. Several model systems were tested: *Yersinia enterocolitica* tissue culture infection; *Klebsiella pneumoniae* tissue culture infection; and animal model infections with *Klebsiella pneumoniae*, *Pseudomonas aeruginosa*, and *Staphylococcus aureus*. Additional studies addressed response of drug-resistant *Klebsiella pneumoniae* to different classes of antibiotics, and bacterial transcriptomics within the context of a mixed biofilm community.

The research applied a novel approach to greatly enrich the representation of bacterial transcripts in mixed libraries, where normally the bacterial pathogen is in very low abundance compared to the eukaryotic host. This, in turn, allows more efficient use of sequencing bandwidth and, as was demonstrated with *Klebsiella pneumoniae*, the technique allowed us to detect low-level expression of genes within the infection model that would otherwise have not been detected using purely brute-force sequencing techniques. The RNA-seq approach is ultimately a hypothesis-generating technique, and the application of our capture enrichment approach improves our ability to generate hypotheses with confidence from complex experiments.



## Modular Abiotic/Biotic Systems (MABS) for Understanding and Directing Biological Function

190960 | Year 1 of 3 | Principal Investigator: C. J. Brinker

### Project Purpose:

This project will create and investigate three classes of modular abiotic/biotic systems (MABS): 1) synthetic biological cells (aka protocells) constructed of synthetic (abiotic) and natural (biotic) components and designed to interact with natural cells, 2) phage scaffolds composed of M13 filamentous phages (selected by *in vivo* phage display to selectively bind to cells or tissues) assembled with nanoparticles and/or protocells into biomolecular nanocomposites with exceptional targeting and internalization characteristics, and 3) nanoparticle decorated/modified bacterial and white blood cells with retained viability and motility but altered phenotypes, cellular interactions, and function. Compared to natural cells and tissues, MABS would be more mechanically and chemically durable and much more chemically complex, incorporating synthetic optical, magnetic, catalytic, electronic, and therapeutic components. In biological settings, MABS could be engineered to detect the onset of cancer or infectious disease as well as selectively deliver customized therapeutic “cocktails” and imaging agents to treat the disease and provide *in vivo* diagnostics of the progress of therapy. Alternatively, MABS could be engineered to be recognized as invading pathogens to illicit an immune response for applications in advanced vaccines, immunotherapy, and wound healing. MABS constructs could potentially enable delivery of cargo to bacteria, mark bacteria for recognition by the immune system or completely disguise bacteria. The modular nature of MABS will enable us to assemble completely new cell and tissue-like materials with artificial and as yet unknown functionalities. MABS constructs will further our ability to engineer and understand the interface between synthetic and natural systems, which is of paramount importance to a broad spectrum of emerging topics in national security and the improved health and well being of the nation.

## Predictive Pathogen Biology: Genome-Based Prediction of Pathogenic Potential and Countermeasures Targets

180814 | Year 2 of 3 | Principal Investigator: J. S. Schoeniger

### Project Purpose:

Pathogens with novel genomes arise from emergence of zoonotic agents, anthropogenic selection, or genetic engineering. Understanding molecular mechanisms of pathogens requires years of work, but arresting an outbreak requires rapid assessment of virulence and countermeasure targets. We are grossly unprepared to respond to an engineered biothreat attack—we cannot cope with naturally emerging drug resistant species. Next Generation Sequencing technology enables rapid availability of complete genome sequences from outbreak-causing pathogens. Large sets ( $N > 100$ ) of genome sequences from taxonomically related pathogens of differing virulence are now publicly available and the cost for sequencing continues to fall. To apply this revolutionary capability to outbreak response, we urgently need better tools to utilize these data to reliably predict pathogenicity, identify pathogen-lethal targets, and predict countermeasure effectiveness.

Currently, best methods predict correct gene function ~60% of the time, and ~30% of bacterial proteins have no assigned function. While improved annotation is necessary, we propose a more fundamental shift to a data-driven comparative approach. We will implement an analysis pipeline wherein gene and genome features are harvested from large sets of related genomes and statistical and machine learning methods are used to predict drug resistance and virulence phenotypes, similar to a Genome Wide Association Study, but with richer feature sets, including horizontal gene transfer descriptors. We will also demonstrate cost-effective sequencing and assembly of hundreds of genomes of common pathogen species directly from clinical samples, and apply our pipeline to predicting observed clinical phenotypes, showing that scaling to ~10,000 genomes will eventually be feasible.

We are attacking a fundamental problem in biology, the prediction of differences in pathogen phenotypes based on differences across a large number of similar genomes. Demonstrating feasibility of sequencing of hundreds of pathogen isolates for which we have clinical data, and comparative analysis using machine learning, will generate new tools for attacking biosecurity problems such as emergence of multidrug resistance.





## Understanding and Engineering Lignolysis for Renewable Chemical Production

173019 | Year 3 of 3 | Principal Investigator: S. Singh

### Project Purpose:

Lignin is the only source of renewable aromatics, and utilization of lignin for high value coproducts will enable biofuel industries to become cost competitive with petrochemicals. The potential US market for a lignin-derived octane enhancer alone is estimated to be 2.2 billion gallons per year. The prospects of macromolecular lignin being utilized as raw materials for fuels and chemicals have been highly touted, but no conversion technologies have been realized. Towards this goal, this project explores two routes: 1) a bio-route based on an engineered organism by borrowing the heterologous enzymes for lignin depolymerization and transportation of the lignin monomers and subsequent modification into value-added chemicals; and 2) a hybrid process—a chemical process followed by a bio-based process that utilizes the engineered organism from the first route.

*Bacillus subtilis* was chosen as a suitable bacterial host for this project as it possesses the ability to secrete the lignolytic enzymes along with other advantages. By performing omics studies on an array of different microbes and substrates, we are aiming to gain knowledge of different transporters involved in lignin uptake, the central metabolism of the lignolytic organism and identify novel enzymes involved in the lignin pathway. We are also evaluating two aromatic transporters from *Rhodopseudomonas* for their capability in uptake of a range of oligomeric compounds derived from lignin. Our final product will be a robust synthetic biology toolbox tailored for lignin, coupled with an engineered microbial chassis that will serve as a springboard for the production of cost-competitive renewable chemicals from lignin.

## Unmasking Hidden Compounds within Hyperspectral Images

190959 | Year 1 of 3 | Principal Investigator: S. M. Anthony

### Project Purpose:

The goal of the project is to reduce the detection limit of weak signal currents hidden within hyperspectral images. While advanced fluorescence microscopy techniques can provide high spatial resolution, high levels of autofluorescence prevent the application of these techniques to many organisms of interest, notably including photosynthetic organisms relevant to bioenergy research. Hyperspectral imaging offers a possible solution, as the spectral information potentially allows the separation of the fluorescent contributions of multiple compounds. However, the existing multivariate curve resolution (MCR) analysis algorithms have difficulty resolving weak spectral components when much stronger spectral components with significant overlap are present. This project seeks to circumvent the current limitations through a combination of hardware and software improvements and demonstrate the relevance of these capabilities in multiple national security mission areas.

On the hardware side, during the course of this project, we will extend the capabilities of Sandia's patented hyperspectral stimulated emission depletion (STED) microscope, configuring it to allow automated setting and scanning of the wavelengths of the excitation and emission lasers. Careful selection of the excitation wavelength will minimize the autofluorescence contributions and increase the flexibility of the hyperspectral STED, allowing its use with a wider range of fluorescent probes. Meanwhile, scanning the wavelength allows excitation-emission mapping, which allows compounds with similar emission spectra to be distinguished based upon their excitation spectra.

On the software side, Sandia's patented MCR algorithms will be updated to improve spectral unmixing. Currently, weak signals are often subsumed by the stronger signals. By accounting for the distribution of the noise and applying appropriate weighting throughout the software processing, the limits of detection should be reduced. Additionally, the software will be updated with rigorous uncertainty quantification capabilities, allowing increased confidence in the results.



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## Computing and Information Science

The Computing and Information Sciences IA champions innovative research and development that advances the state of the art in mathematics, information sciences, and computing relevant to Sandia's national security missions. As these applications continue to technically deepen and broaden (internally and externally), there is an ongoing need to refresh and advance underlying knowledge and capabilities. The scope of the IA includes computer and computational science and engineering, information science (including mathematics and cognitive sciences), and aspects of cyber sciences and data sciences. The IA is pursuing several strategic objectives. First, we want to develop the technologies that will underpin the success of future generations of computers. These technologies include scalable system architectures and software, as well as novel approaches to future machines including quantum, neuro-inspired, and other advanced concepts. Second, we want to advance the mathematics and computational science capabilities that enable high confidence in our modelling and simulation results. Third, we want to develop and apply information science capabilities for Sandia's national security applications. All three of these objectives involve increasing the confidence in critical decisions and considering the human element in our approach to computing.

*The figure above depicts tunnel couplings computed for two phosphorus donors in silicon. One donor was placed at the origin and the second at every possible point within a 30 nanometer cube surrounding it (~1.3 million instances). The spherical shells show cuts (with nearest-neighbor interpolation) of the tunnel coupling at fixed donor separation distances. This work is expected to aid in the experimental realization of qubits that will enable quantum computing. (Project 173883, Scaling up Semiconductor Quantum Computers through Multiscale Analysis)*

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## (Active) Learning on Groups of Data with Information-Theoretic Estimators

181061 | Year 2 of 2 | Principal Investigator: W. P. Kegelmeyer

### Project Purpose:

Machine learning techniques in problem settings such as classification, anomaly detection, and regression typically focus on single points as the unit of interest; the underlying data is projected into a feature space before the algorithms ever see it. This projection, however, is not always natural, and it may discard key information. In many settings, we wish to perform machine learning tasks on objects that best can be viewed as a set of lower-level objects: for example, images can be successfully viewed as a collection of local patches. In order to use traditional techniques on these set-based objects, we must create a single vector that represents the entire set. Though there are various ways to summarize a set as a vector, we can discard less information and potentially require less work in feature engineering by operating directly on sets of feature vectors.

One method for machine learning on sets is to consider them as samples from some unknown underlying probability distribution over feature vectors. Each example has its own distribution: if we are classifying images as sets of patches, each image is defined as a distribution over patch features; each class of images is a set of patch-level feature distributions. We can thus explore kernel methods, based on statistical estimates of distances between probability distributions, to classify samples from these distributions. Because we obtain a kernel, we can exploit the substantial literature of kernel methods to solve many types of learning problems. The work is in collaboration with Carnegie Mellon.

## A Case Study on Neural Inspired Dynamic Memory Management Strategies for High Performance Computing

194773 | Year 1 of 2 | Principal Investigator: C. M. Vineyard

### Project Purpose:

Exascale-class supercomputers will require unprecedented amounts of memory bandwidth and capacity. To satisfy these requirements, vendors are proposing multi-level memory (MLM) combining different memory technologies in a single system. MLM partitioning within compute nodes will become a crucial aspect of achieving high-performance levels. Previous research has quantitatively shown the advantage of user-controlled mapping to multi-level main memory for a class of sorting algorithms with potential applicability to a variety of other computational primitives [Bender et al., IPDPS 2016].

No established methods to dynamically manage MLM partitioning exist. Rather, MLM systems will rely upon application or runtime systems to manage how data is staged between low-bandwidth/high-capacity memory and high-bandwidth/low-capacity memory or depend upon manual mapping. Alternatively, we are proposing to explore the ability of neural inspired dynamic memory management strategies to learn application specific memory management schemes for high performance computing architectures.

To do so, we will begin with the class of sorting algorithms which have been shown to have a beneficial two-level memory mapping [Bender et al., IPDPS 2016], and explore the neural learnability of mapping such algorithms. Furthermore, we seek to identify key characteristics making a neural approach applicable to larger classes of problems so that the applicability of such an approach to DOE codes may be assessed.





## A Framework for Wind Turbine Design under Uncertainty

173867 | Year 3 of 3 | Principal Investigator: M. S. Eldred

### Project Purpose:

Wind energy is an increasingly vital component of the electricity generation system in the United States and by the year 2020 it is expected to compose 10% of the energy portfolio. The only certain thing about this estimate is that it is uncertain. There are numerous uncertainties in wind energy: policy, market, technological, and power production. The uncertainty in power production is caused by the inherent variability of atmospheric wind conditions and by wake effects. We can reduce the power uncertainty by designing wind turbines that properly consider the effects of the uncertain wind conditions on the wind turbines performance.

The optimization of a wind turbine—or group of turbines—is a complex multidisciplinary problem. The aerodynamics discipline is an important component of the analysis and optimization (design) problem. To simulate the aerodynamics of a wind turbine(s), many different aerodynamic models exist where each model has a different fidelity and associated computational cost. It is desired to analyze and design the wind turbines with the highest fidelity model; however, this is unfeasible because of the prohibited computational cost associated with the numerous simulations needed in an optimization under uncertainty. To reduce the cost—while maintaining high-fidelity accuracy—we can use multifidelity methods. These methods combine the results of the models of different fidelity to approximate the highest fidelity model.

In developing the framework for wind turbine design under uncertainty, we have focused on computationally modeling the aerodynamics and the uncertainties that affect the aerodynamics. In particular, we have focused on airfoil (blade) aerodynamics, vertical axis wind turbines operating in extreme uncertain gust conditions, and the optimization of wind farms consisting of horizontal wind turbines.

## Advanced Data Structures for Improved Cyber Resilience and Awareness in Untrusted Environments

180820 | Year 2 of 3 | Principal Investigator: C. A. Phillips

### Project Purpose:

This project focuses on fundamental research in write-optimized data structures (WODS) with application to resilient high-performance data management. We consider data sets so large they must be partially stored on external memory-like disks. WODS enable systems to ingest and index data orders of magnitude faster than with previous data structures. There are write-optimized data structure replacements for B-trees (for data bases) and for Bloom filters (for approximate membership queries). Developed for commercial databases, WODS have not been applied in security settings.

We will create WODS to enable network security monitoring components to stream high-speed network data to disk and/or solid state drives, and perform complex queries on that data during subsequent analyses. The additional speed of WODS, available for cybersecurity for the first time, will create new opportunities to decide what to store and what queries to support. We will add features to WODS to make them more useful for cyberstream monitoring. These include aging data and handling significant data repetition. We will quantify performance improvements on real(istic) cyberstreams. We will consider hash-based data structures, which makes every input pattern behave randomly, and comparison-based data structures, which allow efficient queries to find all keys in a range of values.

We will design data structures that combine the speed of WODS with secure/resilient storage systems. A memory snapshot from history independent (HI) data structures does not reveal anything about the past history of the data structure, such as the order elements were inserted. We will explore fundamental tradeoffs between history independence and data structure performance in both main and external memory.



## Advanced Uncertainty Quantification Methods for Circuit Simulation

173331 | Year 3 of 3 | Principal Investigator: E. R. Keiter

### Project Purpose:

The proposed research aimed to develop advanced uncertainty quantification (UQ) methods for analog circuit simulation, with the goal of mitigating the expense of large ensemble Xyce circuit calculations that result from sampling. The primary output has been the exploration of a set of advanced methods to determine time-dependent UQ of nuclear weapons (NW) circuits. Currently, NW circuit designers and analysts rely almost exclusively on brute-force nested sampling methods, requiring expensive numbers of simulations. Our research has extended reliability and gradient-enhanced regression polynomial chaos expansion (PCE) methods to production level circuit simulation.

The initial focus of this project was on reliability methods, but it was determined during the first year that these were unlikely to be accurate enough for our purposes. We subsequently moved on to studying PCE methods. For both reliability and PCE methods, analytic parameter sensitivities are advantageous, so we performed research and development on circuit sensitivity methods throughout the project. Also, both methods naturally led to field data capabilities being added to Dakota, which is another project accomplishment.

Using gradient-enhanced PCE, we believe that we have successfully demonstrated a significant reduction in the number of simulations required to perform circuit UQ studies. Outputs of interest to NW circuits include circuit metrics such as power-rail collapse, signal delay, and reduction of bipolar transistor gain, while inputs are generally model parameter such as oxide thickness or resistance values. It is anticipated that these new capabilities will impact the Qualification Alternative to Sandia Pulsed Reactor (QASPR), Enhanced Surveillance, and Life Extension Programs (LEPs) among other projects.

Gradient-enhanced PCE had not been previously attempted for production-level circuit simulation. Additionally, fully analytic sensitivities are not available in most (if any) circuit simulators besides Xyce. Our work has resulted in a number of new features in both Xyce and Dakota, which are available in formal code releases.

## Adverse Event Prediction Using Graph-Augmented Temporal Analysis

190965 | Year 1 of 3 | Principal Investigator: R. Brost

### Project Purpose:

This work addresses the difficult problem of searching complex data streams for patterns leading up to adverse events. Given a time series of remote sensing and other data, we propose a method for searching temporal data for precursors leading up to adverse events. This would aid both forensic event analysis and prediction of a possible future event. A key challenge is that for realistic problems there can be an enormous number of possible causal relationships, leading to both computational expense and a potentially overwhelming number of returned false positives. Meanwhile, false negatives also pose a significant challenge.

We propose to address these issues by augmenting the temporal analysis with relationship information inferred from a geospatial-temporal semantic graph. This would reduce computation time, focus output to a relevant subset, and exploit the information content of the graph. We intend to implement and test this approach on a number of examples, including both open and national security data sets.



## Analyst-to-Analyst Variability in Simulation-Based Prediction

173028 | Year 3 of 3 | Principal Investigator: M. R. Glickman

### Project Purpose:

From informal observation and discussions with analysts, we have become aware that, even when provided the same problem, source data, simulation tools and specific questions, it is unlikely that two analysts will arrive at the same predictive judgments. Moreover, in multiple challenge-problem workshops in which teams of professionals have derived probabilistic estimates based upon a common problem scenario, answers have often varied by orders of magnitude.

What impact might uncertainty indicated by this variability have on national security applications? Are there effective ways to mitigate associated risk and/or improve decision making? We don't know because there have been few, if any, formal studies of analyst-to-analyst variability in simulation-based assessment. In lieu of such studies, analyst judgment is developed through professional training and mentoring and subjected to peer review. Despite these practices, there remains a large disparity between our relatively intuitive approach to analyst judgment and our formal treatment of other stages of the simulation-based assessment pipeline such as hardware architectures and numerical algorithms. More alarmingly, psychological research consistently reveals reliable biases in human judgment and decision making, biases that were only divined via formal analysis.

In this study, qualitative studies of simulation-based judgment as practiced at Sandia and elsewhere were used to design a formal experiment in which subjects were presented with a rich, end-to-end uncertainty quantification problem and asked to derive a range of assessments. Results from this experiment are being analyzed to understand how differing assessments may be traced to differing methodological choices or preferences when quantifying uncertainties in a complex, simulation-based predictive analysis, which may in turn be traced to variations in individual beliefs and/or judgments.

## Counter Adversarial Graph Analytics

190966 | Year 1 of 3 | Principal Investigator: W. P. Kegelmeyer

### Project Purpose:

Graph analysis algorithms are a key part addressing problems spanning many national security missions. The key S&T questions are: What vulnerabilities lurk in those algorithms? Can we discover, study, and quantifiably characterize those vulnerabilities under the assumption that they are being exploited by informed, empowered adversaries? Can we develop remediations for those vulnerabilities that aren't, themselves, subject to subversion by an adversary?

To structure our research, we start with deep investigation of two very different graph analysis algorithms with national security applications, and end with an analysis of the general principles that can be gleaned from both.

Specifically, we have begun with "community detection" (CD), which is a means of grouping the nodes of a graph into communities, for subsequent analysis. We assume an adversary that wishes to subvert that community detection, who wishes to insure that a particular node is *\*not\** associated with its correct community. Further, we assume that the adversary has the ability to insert edges to achieve this end. To analyze CD algorithmic vulnerability, in the first year we have:

- Found many CD vulnerabilities, implemented them, and generated copious empirical studies.
- Developed novel mathematical theory around the behavior of communities under attack, and under a "sparsification" defense.
- Developed a novel visualization tool to clarify the nature of the adversary's corruption of the natural community assignments.
- Developed a novel synthetic graph simulation method to support statistically significant assessment of our empirical investigations.

Our research is different from prior research in two primary ways: 1) most "vulnerability assessment" is of the hardware or software implementation of the algorithms; we focus on the vulnerability of the algorithms themselves, and 2) most CD analysis research focuses (inconclusively) on the general properties of the communities or graphs: we directly assess how CD is used as input to a subsequent analytic.





## Coupling Computational Models: From Art to Science

173025 | Year 3 of 3 | Principal Investigator: P. B. Bochev

### Project Purpose:

The purpose of this project was to formulate, develop, implement, and test new numerical methods for interface problems arising in many national security applications. The effort comprised two complementary research tracks: 1) development of partitioned methods for explicit elastodynamics based on mathematically rigorous Lagrange multiplier formulations and 2) application of optimization and control ideas to the solution of transmission and mesh-tying problems.

The main objective of the first track was to develop rigorous mathematical foundations to enable efficient reuse of existing verified and tested codes for the simulation of structure-structure interaction problems, which is particularly important for nuclear weapon impact sensors. Providing such sensors for contemporary systems requires solution of coupled problems for the sensor and the rest of the system. Currently this task is accomplished by using Sandia's Sierra/SM and Alegria codes under the restriction of a matching nodes interface, which can reduce the efficiency of the overall simulation. The Lagrange-multiplier-based partitioned methods resulting from this work are applicable to general interface configurations and have the potential to improve the efficiency in this and other mission problems.

The second research track represented a forward looking effort aiming to demonstrate the applicability of optimization approaches for the solution of coupled and interface problems. One aspect of this work explored optimization-based methods for problems with spatially non-coincident interfaces that arise when a curved interface is meshed by, e.g., affine simplex elements. Another aspect explored optimization-based formulations for heterogeneous numerical methods (i.e., methods comprising numerical and/or mathematical models with fundamentally different properties such as local and nonlocal continuum models).

## Data-Driven Optimization for the Design and Control of Large-Scale Systems

180822 | Year 2 of 2 | Principal Investigator: D. P. Kouri

### Project Purpose:

Engineering decisions are often formulated as optimization problems constrained by large-scale physical simulations involving partial differential equations, ordinary differential equations, and differential algebraic equations. In such problems, the governing simulations typically involve uncertain input parameters (e.g., loads and materials), unknown initial and boundary conditions, and unverifiable modeling assumptions. An example application is the reliability testing of components using direct field acoustic testing (DFAT). In DFAT, one must determine loud speaker output that reproduces target vibration profiles through the component while accounting for material uncertainties. Another application is to design an elastic structure that is resilient to a variety of external loads or to internal residual stresses. For such problems, the underlying probabilistic characterization of the uncertain inputs is typically unknown, but estimated from noisy and incomplete data (e.g., residual stress in elastic design). In these situations, it is critical that the optimal solutions are robust to this "distributional" uncertainty.

*The goal of this project is to fuse data, uncertainty and simulation in novel algorithms and discretizations for the rapid and robust solution of mission-critical optimization problems.*

A common approach for formulating and solving these problems is to assume a known probability distribution for the uncertain parameters, discretize the governing dynamics using standard numerical approximation schemes, and solve the resulting finite-dimensional optimization problem. In many applications, such as reliability engineering, assuming a known probability distribution can lead to unreliable system performance with potentially catastrophic outcomes. To circumvent this issue, we developed novel discretizations and optimization formulations that do not assume a known probability distribution, but rather use data to determine an optimal solution that is robust to our ignorance of the true probabilistic characterization of the uncertain inputs. The outcome of this project is a rigorous and broadly applicable framework for optimal design, control, and decision making in the presence of uncertainty that combines data, simulation, and optimization.



## Dynamical Systems for Resilient Computing

198384 | Year 1 of 1 | Principal Investigator: F. Rothganger

### Project Purpose:

The effort to develop larger-scale computing systems introduces a set of related challenges. Large machines are more difficult to synchronize. The sheer quantity of hardware introduces more opportunities for errors. New approaches to hardware, such as low-energy or neuromorphic devices are not directly programmable by traditional methods.

These three challenges may be addressed, at least for a subset of interesting problems, by a dynamical systems approach. The initial state of system represents the problem, and the final state of the system represents the solution. By carefully controlling the attractive basin of the system, we can move it between these two points while tolerating errors, which appear as perturbations.

Numerical continuation is a technique amenable to this form, as it involves following a manifold while some controlled parameter varies. A wide range of interesting numerical problems have continuation formulations worked out in the literature. We ask two key questions (1) Can a continuation formulation provide more resilience to errors on conventional computing hardware? If so, does the additional cost justify using the technique? (2) Can these be solved using a dynamical system rather than the usual predictor-corrector approach?

## Game Theory for Proactive Dynamic Defense and Attack Mitigation in Cyber-Physical Systems

177965 | Year 3 of 3 | Principal Investigator: J. Letchford

### Project Purpose:

Malicious attacks on cyber-physical systems, such as nuclear weapon systems or the electric power grid, are orchestrated by human attackers whose decisions are influenced by personal incentives. Current systems take into account that the value of a security system or policy is not only in the attacks that it successfully foils, but also in the way that potential attackers' actions are changed. However, there are many other (non-accounted) decisions already being made in these systems that also have the potential for deterring attacks. For example, strategies for mitigating the extent of system failure or backup systems ignore this deterrence effect, and are not included in current security models. When our security and resilience models ignore the changes in attacker incentives due to other investment areas, we are less effective in allocating our limited resources. Our goal is to develop models and algorithms that manage the computational issues that arise when we consider a wide range of potential deterrence effects and enable more efficient planning for investments in security, resiliency and mitigation, both exploiting potential synergies and avoiding costly redundant investments.

We will use adversarial game theoretic analysis to develop new models and algorithms for cyber-physical systems that characterize the deterrence factor of infrastructure investments that make attacks impossible, and of investments that reduce the impact of system failures. We will develop the first models that take into account the interconnected nature of these investment areas.



## Graph Learning in Knowledge Bases

183780 | Year 2 of 3 | Principal Investigator: A. Pinar

### Project Purpose:

Data science has continued to become a foundational pillar to many national security research applications. Current science and technology approaches to data science focus on post-acquisition analysis. Very few analysis techniques support the data acquisition process itself. This research hopes to move the state of the art closer to a framework that allows for quantitative assessment of the value of data to the problem being solved (also known as “data valuation”).

This problem is trivial if all data were equally valuable and useful, but this is not the case in practice. Data elements can have complex relational dependencies where some aspects of the data can be inferred, making its physical acquisition redundant. This inference is inherently probabilistic and maintaining data in this form requires a knowledge base structure that can handle nondeterministic queries. In contrast, traditional database queries return a single answer (requested data or null), which hampers in absentia use of inferred data. To address this problem requires advances in probabilistic knowledge bases and their utilization.

The goal of this research is to leverage (and advance where necessary) recent advances in state-of-the-art probabilistic knowledge base design and couple them with statistical inference and learning algorithms. More specifically, probabilistic knowledge bases report per cell a probability indicating the likelihood that the element is a particular value. Furthermore, to be more integrated with mission requirements, these techniques will attempt to address issues and opportunities created with human-in-the-loop analysis patterns and techniques.

This work is in collaboration with the University of Florida.

## Heimdallr: Automated Binary Analysis via Symbolic Execution

190964 | Year 1 of 2 | Principal Investigator: C. B. Harrison

### Project Purpose:

Malware proliferation is growing exponentially; current defensive techniques are overwhelmed by the volume and, increasingly, the sophistication, of the malicious programs. Traditional techniques, notably reverse engineering, require onerous time investment from a small pool of highly skilled individuals. This has led to a growing asymmetry between attackers, who can easily and automatically obfuscate their programs, and defenders that must be addressed.

We propose to address this asymmetry using symbolic execution (SE) to automatically reverse engineer malicious programs and output salient information. Specifically, SE executes programs with symbolic inputs and forks execution at every branch condition to explore all paths through a program. Once the SE engine reaches a state of interest, it can then examine the tree of branches to determine a concrete set of inputs that satisfy all the branch conditions leading to that state of interest. This technique has numerous applications including malware analysis, vulnerability analysis, program optimization, and test code generation. Our goal is to develop an SE engine that: 1) increases the scalability of symbolic execution of malware, and 2) aids reverse engineers by automatically reverse engineering the protocols used by arbitrary malicious program.

SE has been successfully applied in prior work to analyze binaries, both benign and malicious. However, existing solutions have numerous limitations and/or have not been made available to the research community. We aim to address these limitations by developing a hybrid static and dynamic SE engine and applying it to problem spaces that relate to various national security mission areas.





## High Performance Computing Metrics to Enable Application-Platform Communication

196223 | Year 1 of 1 | Principal Investigator: A. M. Agelastos

### Project Purpose:

Emerging high performance computing (HPC) platforms continue to increase in processing elements along with interconnect and file-system bandwidth. While the cycle for a new platform is around five years, developers are continuously tuning algorithms and methods to utilize all platform resources and maximize performance. Thus, a new system's shared resources are rapidly taken advantage of and easily oversubscribed. Though a particular application's constituent parts may operate in harmony with respect to available resources, there are currently no mechanisms to enable competing applications to load balance. Therefore, performance-crippling contention often occurs which can lead to platform instability if competing applications' cumulative needs exceed the platform's capabilities.

The goal of this work is to enable balanced platform resource usage while minimizing/bounding resource contention. We took the novel approach of using whole system high fidelity monitoring to identify metric definitions that can be used as meaningful actionable indicators of performance-affecting contention. Currently, the identification of such indicators and the quantification of resultant performance impact is largely unknown.

In this work, we defined and verified a set of metrics pertaining to network and file-system resources that quantify the extent of the resources' utilization/congestion. We examined performance and resource utilization/contention of CTH, Sandia's shock physics analysis system, IMB (network benchmark), and IOR (file-system benchmark) using Sandia's Lightweight Distributed Metric Service (LDMS) for monitoring state data on Mutrino, a test system for Trinity (the latest DOE NNSA Advanced Technology System). We researched methods to distill LDMS data into actionable metrics that can be provided to application developers and used for run-time resource management. We created an Actionable Metric Model, through controlled testing, verification, and modeling, that was used to quantify the time during, and slowdown from, contention.

## Identification of Markers of High RANS Uncertainty for Model Improvement in Engineering Flows

180823 | Year 2 of 3 | Principal Investigator: J. Ling

### Project Purpose:

The purpose of this project is to develop and apply machine learning techniques for the detection of regions of high model form uncertainty in Reynolds Averaged Navier Stokes (RANS) flow predictions. RANS simulations rely on empirical transport equations to model transport due to turbulence. These simulations are susceptible to high uncertainty when the underlying model assumptions are violated. Current methods for validating RANS simulations rely on validation experiments or high fidelity simulations, both of which can be costly or infeasible to perform for many flows of engineering relevance. Therefore, there exists significant demand for computationally efficient methods that can detect regions of high model form uncertainty in RANS simulations.

Machine learning algorithms are data-driven methods that can leverage the big data generated by computational fluid dynamics simulations to learn when RANS model assumptions are violated. These algorithms are trained on a database of canonical flow configurations for which both high fidelity and RANS results are available. These detectors for elevated RANS uncertainty have a range of potential applications. They are immediately useful for post-processing simulation results because they enable users to know in which regions of the flow their simulations have increased uncertainty. Furthermore, they could be used to trigger adaptive corrections during run-time. They are also informative in experimental design to designate the regions of the flow that should be probed to provide the strongest validation for the simulation results.

This research represents a high-risk, high-reward endeavor. New techniques are sought for embedding domain knowledge into machine learning algorithms, for translating algorithmic predictions into physical rules, and for enabling adaptive corrections during run-time based on machine learning predictions. All of these advances would represent significant leaps from the current state of the art.



## In Situ Compressed Sampling and Reconstruction of Exascale Unstructured Mesh Datasets

180818 | Year 2 of 3 | Principal Investigator: M. Salloum

### Project Purpose:

Post-Moore and exascale platforms are expected to generate datasets that are too large to be reliably stored or transferred across networks, thus impeding data exploration and knowledge discovery. In situ data compression can address this problem, but current efforts are overwhelmingly targeted at data defined on regular lattices. These efforts are not suitable for data defined on irregularly spaced points—"point-clouds"—(e.g., unstructured meshes).

We will develop a fast data compression method for time-dependent fields defined on point-clouds. It will be based on the theory of compressive sensing (CS) of videostreams. Conventional CS theory, developed for image compression, is based on the representation of lattice data using first generation wavelets. We will extend the theory to encompass second generation wavelets (SGW) that can be described on point-clouds. This extension will require designing random matrices that are incoherent with SGW and establishing the restricted isometry required for unique inflation of compressed samples. Time-series modeling of wavelet representations of datasets will be used to reduce the temporal reconstruction cost. We will also investigate scalable reconstruction algorithms and error metrics to be combined into a practical framework for analysis and knowledge discovery.

Our method will be implemented as a parallel codec (coder/decoder) and demonstrated in compressing/inflating a time-dependent, 10-billion-node dataset from a turbulent jet simulation running on Cielo. Such data compression capability will be of relevance to exascale engineering simulations conducted for nuclear weapons and energy efficiency applications. The cloud-of-points data representation will also make the codec applicable to particle-based simulations.

## Modeling Human Comprehension of Data Visualizations

190967 | Year 1 of 2 | Principal Investigator: L. E. Matzen

### Project Purpose:

A key factor in designing effective algorithms and tools is presenting the data to the human user in a format that s/he can interpret and understand. Visualizations are a common way to present data to users because humans rely heavily on vision to navigate the world, and those same cognitive processes can be used to navigate through information space. However, as data sets and analyses become ever more complicated, presenting information to analysts in a way that they can comprehend becomes ever more challenging.

While there is a great deal of research devoted to data visualization methods and techniques, efforts to assess the effectiveness of the resulting visualizations for the end users remain rare. Prominent researchers have argued that "the creation of comprehensive models of human-computer cognitive processing should be a core component of the visual analytics effort, and is an essential prerequisite for success of visual analytics as a field." We are building such a model by combining a bottom-up model of visual saliency with top-down eye tracking studies of sensemaking. This novel combination of evaluation and modeling techniques drawn from the cognitive science and information visualization literature will lay the scientific foundation for evaluating data visualizations from a human cognitive perspective. Understanding both *what* attracts a user's attention and *why* will place us on stronger footing for designing more effective visual representations. With data complexity far outstripping the power of our representations, this ability constitutes a strategic advantage as well as a deep theoretical contribution.

This project will build on Sandia's unique combination of strengths in data science, cognitive science, and information visualization to address fundamental questions about comprehension of abstract data visualizations. These questions are critically important for advancing the field of visual analytics and for improving human performance in the numerous mission areas that rely upon visualizations to support analysis and decision making.



## Modeling Information Multiplexing in the Hippocampus

178470 | Year 3 of 3 | Principal Investigator: F. S. Chance

### Project Purpose:

Modern computers face the challenge of processing ever-growing quantities of data that span a wide range of modalities. Of particular relevance to national security interests is the ability of sensor systems to integrate multimodal data for the purpose of fast and automated decision making. The brain is a biological system that is specialized for high performance at this task, suggesting that understanding the mechanisms by which neural circuits integrate multimodal data may lead to improved automated detection systems. This research project will develop and test a novel theory of how neurons in the hippocampus integrate, process, and transmit different information streams. Our goals were to: 1) test the hypothesis that hippocampal neurons multiplex information from two different input streams and 2) generate a description of this multiplexing algorithm that will be implementable in computer systems. If this hypothesis is verified, this research will be the first demonstration (to our knowledge) of multiplexing in any nervous system. Successful outcomes could aid the development of new brain-inspired algorithms for multimodal data integration. These algorithms could significantly impact brain-inspired Beyond Moore computing research at Sandia and enhance data processing systems vital for the national security missions of Sandia and the DOE.

## Next-Generation Electronic Structure Codes for National Security Application

195213 | Year 1 of 1 | Principal Investigator: L. Shulenburger

### Project Purpose:

First principles calculations of material properties are an invaluable tool in fields as diverse as materials science, chemistry, and plasma physics. These methods combine relatively modest computational cost with high fidelity, even when applied to materials or conditions that are novel or extreme. Their extraordinary success has, in turn, driven research into improved approximations and novel algorithms that promise to dramatically expand the already broad application of these methods into new areas of great interest to the national security community.

However, the codes and algorithms that are currently employed were designed and implemented in an era of more primitive approximations and simpler computer hardware and are limited to super cells consisting of on the order of approximately one hundred atoms. These limitations have restricted the application of density functional theory (DFT) to fairly simple compositions and stoichiometric alloys.

This project explored theoretical and computational algorithms to dramatically expand the applicability of DFT, including advances in approximations, algorithms, and computer architecture to enable DFT calculations of more complex materials.

While many DFT codes exist, none of the projects behind them are aimed at developing a community code that is flexible and widely applicable to both high performance computing platforms and materials technologies. Developing such a code requires algorithmic innovations. This project demonstrated this assertion and provided analysis of algorithms to meet this need while also identifying several topics for which future development is needed.





## Optimal Control and Design of Qubits

190970 | Year 1 of 3 | Principal Investigator: G. J. Von Winckel

### Project Purpose:

Quantum computers offer immense potential for applications in cryptography, factorization, and exhaustive search methods. One of the most promising implementations for quantum bits (qubits), leading to a scalable computer, is based on nanoscale placement of donor atoms into a silicon substrate. While there has been some work in recent years involving quantum control with Lindblad constraints, typically this has been problem specific and used nonoptimized codes. This project aims to develop a computational infrastructure to aid in the design of and establish optimal operating characteristics for donor qubit devices that will extend upon existing capabilities in Quantum Computer Aided Design (QCAD), which is built on top of Sandia's AgileComponent software framework.

We plan to incorporate the multi-valley effective mass model into QCAD and develop an interface to the Rapid Optimization Library. With these tools, we will solve both steady-state and dynamical problems that impact qubit performance to allow for state-of-the-art design and control. In the steady-state regime, we will formulate and solve inverse eigenvalue problems wherein the lowest energy levels of a donor qubit which are governed by self-consistent Schroedinger-Poisson with a Thomas-Fermi energy functional. The goal will be to compute gate dimensions and locations which yield desired energy levels over applied bias. In the dynamic case, we will project onto a suitable bias-dependent eigenbasis and use the governing equation (Schroedinger, Lindblad, etc.) as an equality constraint to compute voltage schedules which yield optimal metrics such as fidelity, coherence, and switching time. Realistic device design and control optimization of donor qubits with multi-valley using high performance computing tools is a novel undertaking and essential part of developing next generation devices for scalable quantum computing.

## PIMS: Memristor-Based Processing-in-Memory-and-Storage

180819 | Year 2 of 3 | Principal Investigator: J. Cook

### Project Purpose:

Continued progress in computing has augmented the quest for higher performance with a new quest for higher energy efficiency. This has led to the re-emergence of processing-in-memory (PIM) architectures that offer higher density and performance with some boost in energy efficiency. Past PIM work either integrated a standard CPU with a conventional dynamic RAM to improve the CPU-memory link, or used a bit-level processor with single instruction multiple data (SIMD) control, but neither matched the energy consumption of the memory to the computation. We propose to develop a new architecture derived from PIM that more effectively addresses energy efficiency for high performance scientific, data analytics, and neuromorphic applications. Our PIM innovation uses intermediate-sized multiple instruction multiple data (MIMD) arithmetic/logic units (ALUs) that match the power consumption of an advanced storage array to maximize energy efficiency. By augmenting storage (instead of memory), the system can address both in-memory computation and applications that access larger data sets directly from storage, hence processing-in-memory-and-storage (PIMS). We will design the PIMS architecture and evaluate the performance/energy tradeoffs for Sandia-relevant applications by developing: 1) a high-level abstraction of PIMS for implementation within existing codes to functionally evaluate performance, 2) an analytic and/or functional PIMS model to investigate architecture performance/power tradeoffs, and 3) a low-level hardware model that provides latency and power data to inform the architecture model. The key challenge will be defining ALU functions (e.g., matrix operations, searching) that adequately support applications, balance memory array and computational energy, and raise system performance.



## Quantum Optimization and Approximation Algorithms

190963 | Year 1 of 3 | Principal Investigator: O. D. Parekh

### Project Purpose:

Quantum algorithms that make use of Sandia's world-class quantum hardware development are essential but scarce. In the 20 years since Shor's groundbreaking quantum algorithm for integer factoring, only a handful of new quantum algorithms, generally providing very modest advantages, have been invented. We propose to remedy this situation by developing efficient quantum approximation algorithms (QAAs) that direct the power of quantum computing toward new mission-driven problems where quantum resources provide *higher quality solutions* instead of *faster run times*.

For many problems whose optimal solutions are hard to compute, there exist elegant *approximation algorithms* that efficiently find solutions that (in a mathematically provable sense) are close in quality to an optimal solution. As one of the oldest methods for coping with hard problems, efficient classical approximation algorithms have been developed for hundreds of problems over the last 40 years. Surprisingly, quantum algorithms research has barely scratched this surface, with only one recent known algorithm qualifying as a QAA.

The main challenge to QAA development is that an optimal solution cannot be computed efficiently; a QAA must both provide a possibly nonconstructive bound on the quality of any solution, and generate a suboptimal solution close to this bound. Classical approximation algorithms rely on convex programming as an amazingly consistent and powerful source of high quality bounds. No analogous quantum tools exist – yet. We will: 1) develop new quantum techniques providing strong bounds and 2) leverage them to devise new QAAs that provide provably better solutions than any known polynomial-time classical algorithms.

Our project is ambitious, requiring intimate knowledge of both continuous and discrete optimization as well as quantum-algorithmic techniques. Sandia is one of the only places where world-class quantum information and optimization experts are interfacing to develop a shared language. Quantum optimization has not even entered its infancy, and we propose foundational work with potentially field-shaping impact.

## Reducing Computation and Communication in Scientific Computing: Connecting Theory to Practice

173882 | Year 3 of 3 | Principal Investigator: G. Ballard

### Project Purpose:

The gap between the peak capabilities of computer hardware and the achieved performance of numerical computations is caused in large part by the high cost of communication (i.e., the movement of data between processors and throughout the memory hierarchy of a single processor). "Standard"  $O(n^3)$  matrix multiplication is the most fundamental dense matrix computation. "Fast"  $O(n^p)$  with  $p < 3$  matrix multiplication algorithms have been identified for over 40 years and are starting to become practical as communication costs dominate. The primary objective of this research is to find an algorithm that is both theoretically and experimentally faster than current implementations (i.e.,  $O(n^p)$  with  $p < 2.81$ ). The secondary objective is to pursue several complementary projects that involve developing other communication-optimal algorithms.

Many researchers have tried to improve the exponent of matrix multiplication, though they were not as concerned with finding a practical algorithm. We propose to use computer-aided search to find a practical algorithm by formulating the problem as an integer-valued tensor decomposition problem. However, the main difficulty is that the problem to solve is nondeterministic polynomial time (NP)-complete.

If the project is successful, the immediate reward will be improvement in applications like the coupled cluster method, a quantum chemistry computation where nearly all the computational time is spent in dense matrix multiplication. In addition, many efficient numerical linear algebra and combinatorial algorithms have been reduced to matrix multiplication, thereby inheriting the best-known complexity. By delivering a fast, practical matrix multiplication algorithm, we can connect all those theoretical results to practical implementations. We will use computer-aided search to find an explicit algorithm and discover an improved method of matrix multiplication by formulating the problem as an integer-valued tensor decomposition problem. The goal is to increase the efficiency of matrix-matrix multiplication.



## Scaling up Semiconductor Quantum Computers through Multiscale Analysis

173883 | Year 3 of 3 | Principal Investigator: J. K. Gamble, IV

### Project Purpose:

Quantum computers have the capability to revolutionize the computation landscape in ways that incremental improvements to conventional computers cannot achieve. Although researchers have had recent success with small-scale devices in many architectures, the largest universal quantum computer demonstrated to date consists of 14 qubits, compared to the billions of bits found in classical computers. It is clear that, for quantum computers to have an impact, they must be massively scaled up.

In this project, we put forward a plan for scalable quantum computation in semiconductor systems. By completing this course of research, we will bring Si-based quantum computing technologies closer to the level of GaAs in terms of device reliability, while sidestepping the decoherence problems intrinsic to GaAs. In stage 1, we will begin by continuing to clarify the role that disorder plays in quantum control of semiconductor qubits. We will develop and validate multiscale effective mass models that phenomenologically incorporate disorder. In stage 2, we will incorporate the results from stage 1 into large-scale models, which are capable of simulating entire devices, and have not yet been able to capture such small-scale features. Finally, in stage 3, we will optimize device designs in order to mitigate the role of disorder. In doing so, the research will help to overcome one of the major obstacles to scalable quantum computing.

The focus of this project is understanding the fundamental science of disordered semiconductor systems. Once the basic science is understood, the knowledge gained will be used to facilitate engineering advances in the semiconductor qubit development Sandia is currently investigating.

## Simulation Capability and Computational Assessment of Memristors as Beyond-CMOS Logic and Memory Devices

173024 | Year 3 of 3 | Principal Investigator: D. Mamaluy

### Project Purpose:

Transition metal oxide (TMO) memristors have recently attracted special attention from the semiconductor industry and academia. Memristors are one of the strongest candidates to replace flash, possibly dynamic random access memory, and static random access memory in the near future.

The purpose of this project is to create a Memristor Charge Transport Simulator that will facilitate understanding of switching mechanisms, predict electrical characteristics, and aid experimentalists in device optimization for different applications. Switching in these devices involves a complex process of oxygen vacancy motion in the TMO film, governed by thermally and electrically driven processes intertwined temporally and spatially.

We have created a memristor simulator that solves, simultaneously, the coupled differential equations: the time-dependent drift-diffusion equations for electrons, holes, and ions/vacancies; the time-dependent lattice heat equation; and the Poisson equation for all the charged species in three spatial dimensions. The drift-diffusion equation for each species includes field drift currents due to electric potential gradients, concentration gradients (Fickian diffusion), and temperature gradients (Soret effect). The heat equation contains Joule heating contributions from all the species. The Simulator will greatly aid Sandia experimentalists in device optimization for different applications.



## Subsystem Reduced-Order Modeling and Network Uncertainty Quantification for Rapid, Agile, Extreme-Scale Simulation

190968 | Year 1 of 3 | Principal Investigator: K. T. Carlberg

### Project Purpose:

Our goal is to enable rapid, scalable simulation of decomposable systems while modeling and controlling system-level uncertainties. We propose to accomplish this by a 'divide-and-conquer' approach that: 1) models the system as a network of subsystems, 2) performs rapid uncertainty analysis via reduced-order modeling (ROM) for each subsystem, and 3) couples subsystem uncertainties via network uncertainty quantification (UQ).

For extreme-scale decomposable systems, high-fidelity simulation and UQ are typically achievable at the subsystem level, but intractable for the full system. This is due to long full-system simulation times, limits on the problem size that can be reliably simulated, and challenges in integrating subsystem models characterized by different physics or scales. Even full-system surrogate models, which are typically employed to make UQ tractable, may not be possible to construct, as they rely on a 'training set' of these (possibly infeasible) simulations.

To this end, we propose a scalable 'bottom-up' approach that performs extensive uncertainty quantification and model reduction at the (tractable) subsystem level, and propagates coupling information using new techniques inspired by domain decomposition. This approach is promising because: 1) full-system ROMs and UQ analyses can be realized without any full-system simulations, 2) network UQ enables full-system uncertainties to be attributed to local contributions for targeted uncertainty reduction, and 3) it enables agile 'Lego-like' analysis and design.

While many mission-critical applications are characterized by decomposable systems (e.g., power systems), our target application will be gas-transfer systems, where full-system qualification is hampered by the intractability of full-system computational fluid dynamics modeling.

We will develop a novel network UQ methodology. If successful, this work will enable a fundamental and broad impact capability for scalable ModSim and UQ of decomposable systems. Sandia is the ideal location to conduct this research, as the work requires a unique combination of expertise in the diverse areas of reduced-order modeling, UQ, high-fidelity modeling, and large scale applications.

## Topological Design Optimization of Convolute in Next Generation Pulsed Power Devices

180821 | Year 2 of 3 | Principal Investigator: E. C. Cyr

### Project Purpose:

We propose novel topology optimization approaches for electromagnetic and plasma systems. If successful, this project would be a first of its kind capability to design the "convolute" structure that couples pulsed power generators to the fusion target in Sandia's Z machine. To date, convolute designs can suffer from substantial (20%) power loss, an issue that is aggravated with increasing voltage, current, and load impedance. Within the 2017 time frame, an improved convolute design is desired. Already progress has been made in understanding and improving physical models of the convolute. In addition, modelers have attempted to reduce power loss through parameterized shape optimization of the convolute and concluded that simultaneous investments in modeling, simulation, and optimization are required.

Our differentiating approach is to develop computational techniques for topology optimization capable of designing a convolute structure that minimizes current loss. The complexity of the convolute physics, dominated by plasma models, will require substantial development of: 1) optimization formulations that support complex 3D topologies, 2) nonlinear programming techniques that improve the convergence of topology optimization algorithms, and 3) multiphysics solution methods that support large jumps in material coefficients. Each of these topics is a substantial challenge in its own right and designing the convolute will require concurrent development of these technologies. If successful, the proposed technologies will lead to an improved convolute design. Moreover, the optimization and solution technology will be applicable to similar plasma physics and multiphysics applications that permeate DOE national security missions.





## Towards Rigorous Multiphysics Shock-Hydro Capabilities for Predictive Computational Analysis

173026 | Year 3 of 3 | Principal Investigator: J. N. Shadid

### Project Purpose:

A number of critical science and weapons applications require predictive analysis of complex shock hydrodynamics with electromagnetics. The physical mechanisms include wave phenomena, material transport, diffusion, chemical reactions, and electromagnetics. The highly nonlinear multiple-time and length-scale response of these systems includes discontinuities formed from shocks, contact surfaces, and complex tabular equations-of-state. Current computational solution strategies use ad hoc combinations of operator-splitting, semi-implicit, and explicit time-integration methods and decoupled nonlinear solvers. The mathematical structure of these methods has not provided stability, accuracy, and efficiency to resolve all the dynamical time scales of interest, nor has it enabled integrated fast sensitivity analysis and uncertainty quantification (UQ).

We will develop a unique, modern, mathematical/computational approach for multiphysics shock-hydro that integrates efficient sensitivity and UQ analysis techniques for specific scientific quantities of interest (QoI) that are required outputs from the forward simulation. Our approach is to develop a well-structured, high-level mathematical model employing recent implicit-explicit time-integration methods and new robust arbitrary-Lagrangian-Eulerian spatial-discretizations. This will enable development of fast adjoint-enhanced integrated sensitivity and UQ methods. Achieving this will require developing: 1) a new general space-time discretization algorithmic framework for stable, accurate, and efficient multiphysics shock-hydro forward solutions that provides for adjoint-enhanced sensitivity and UQ (moderate-to-high-risk) and 2) robust adjoint-based techniques for: sensitivity analysis, surrogate model creation for UQ, numerical error estimation, and methods to detect and handle discontinuities in QoI over parameter-space (high risk). To guide and challenge this effort, the exploding wire will be our focused multiphysics shock-hydro application.

## Understanding the Hierarchy of Dense Subgraphs in Stationary and Temporally Varying Setting

194774 | Year 1 of 2 | Principal Investigator: A. E. Sariyuce

### Project Purpose:

Graphs are widely used in many applications of national security such as cybersecurity, nonproliferation, critical infrastructure protection, counterterrorism, and counterintelligence. A common property of graphs arising in these applications is that while the graphs are globally sparse, vertex neighborhood subgraphs are often dense. Finding these dense regions of the graph is the basis for finding anomalies or identifying functional units, and is one of the fundamental problems in graph analysis. Thus, this project aims to develop methods to identify dense regions of a graph when the edges of the graph are updated in a stream.

The underlying algorithmic challenge with finding dense graphs is that most standard formulations of this problem (like clique, quasi-clique, k-densest subgraph) are NP-hard. Furthermore, current dense subgraph-finding algorithms usually optimize some objective in stationary settings, and only find a few such subgraphs without providing any structural relations among them. However, the goal is rarely to find the "true optimum," but to identify many (if not all) dense substructures in stationary and dynamic scenarios, understand their distribution in the graph, and ideally determine relationships among them. We aim to devise algorithms and present visualizations to find the hierarchy structure between dense subgraphs in stationary and dynamic settings, and then understand the structure of the hierarchy to gain more insight on the hidden patterns in real-world networks. We plan to study the stationary scenario first where the entire graph is known, and then switch to the dynamic scenario where the graph is temporally varying.

Finding dense subgraphs with varying densities and sizes, and building a hierarchy among them should be done in linear time; existing algorithms are incapable of these requirements. Furthermore, the dynamic nature of networks requires adaptation of those nonexistent linear (or sublinear) algorithms. We propose to use peeling algorithms and the recently introduced nucleus decomposition framework to attack this problem.



## User-Accessible Unified Manycore Performance-Portable Programming Model

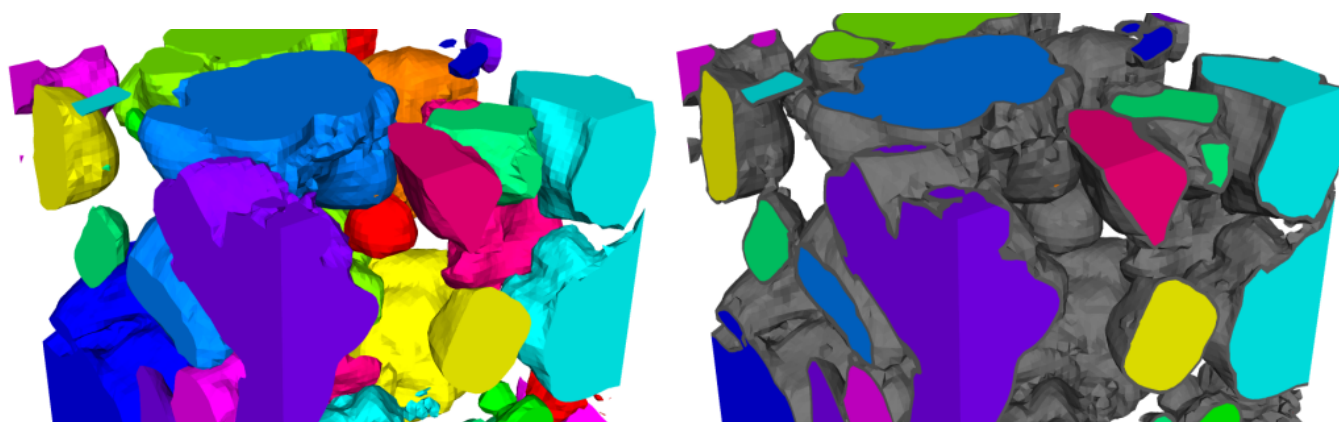
173029 | Year 3 of 3 | Principal Investigator: H. C. Edwards

### Project Purpose:

Rapid and disruptive changes in computing architectures (i.e., the manycore revolution) impact DOE/NNSA mission-critical computational science and engineering codes. The diversity and ongoing evolution of architectures undermines portability of these codes, and code teams typically lack resources and expertise to migrate their codes to multiple, changing manycore architectures (e.g., terascale workstations, petascale clusters, and exascale supercomputers). Migrating applications to manycore architectures currently requires scientists and engineers to have detailed knowledge of vendor-specific performance characteristics and constraints, obfuscate essential mathematics in their codes with parallel processing directives, and generate and maintain multiple versions of codes to meet vendor-specific performance requirements. Even vendor-neutral programming models (OpenMP, OpenACC, OpenCL) require architecture-specific knowledge to achieve acceptable performance and pollute mathematical code with parallel processing directives.

Two key Sandia R&D products are addressing independent facets of manycore parallelism. Qthreads addresses task parallelism with highly efficient task scheduling algorithms. Kokkos addresses data and vector parallelism through a performance-portable interface that minimizes users' exposure to architecture-specific details. We plan to integrate these R&D efforts to create a unified, user-accessible manycore performance-portable programming model for the complete range of manycore parallelism: task, data, and vector. Our qualitative user accessibility goal is to allow scientists and engineers to program emerging manycore architectures with neither extensive architecture-specific knowledge nor ubiquitous parallel processing directives.

Merging these disparate and cutting edge tracks of R&D into a programming model that minimizes teams' demand for manycore expertise (user accessible), minimizes codes' need for architecture-specificity (performance portable), and maximizes opportunities for manycore scalability (task-data-vector parallelism) is an extreme challenge unmet by any past and current R&D efforts. The new programming model provides a clear and cost-effective path forward for our broad set of mission-critical analysis codes to meet the disruptive, ongoing manycore revolution in computer architectures.



## Engineering Sciences

The Engineering Sciences Research Foundation (ESRF) drives understanding and innovation by integrating theory, computational simulation, and experimental discovery and validation to understand and predict the behavior of complex physical phenomena and systems. The ESRF Investment Area supports innovative, leading-edge R&D that: 1) advances the scientific understanding of physical phenomena underlying problems of interest to Sandia, 2) drives innovation and broad usage of state-of-the-art, validated computational modeling and simulation tools, and 3) accelerates the development of experimental diagnostics for discovery, model validation, and enhancement of our test and evaluation capabilities.

*The figure above depicts a simulation mesh reconstructed from a real lithium cobalt oxide battery cathode, where active material is shown in color and polymer:carbon black binder is shown in gray. This research will give us a critical new capability to understand performance, margin, and safety of rechargeable lithium batteries, which are used in a variety of national security applications. (Project 173098, Mechanics of Battery Degradation through Stress Driven Rearrangement of Percolated Conductive Networks during Discharge and Cycling)*

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## A Mesh-Free Method to Predictively Simulate Solid-to-Liquid Phase Transitions in Abnormal Thermal Environments

173194 | Year 3 of 3 | Principal Investigator: J. A. Templeton

### Project Purpose:

Metal melting and encapsulant decomposition significantly impact weapon systems' safety in abnormal thermal environments. Currently, Sandia has no production-ready simulation capability to predict system failure due to complex thermal-mechanical processes or provide the computational verification and validation required to confidently assess associated nuclear safety issues. Most existing finite element codes are also unable to adequately capture massive geometry changes and liquid relocation. Alternatively, Smooth-Particle Hydrodynamics has been applied to molten aluminum flows (Prakash, 2009), but its formulation precludes phase changes and uncertainty quantification. Other particle formulations, such as the Reproducing Kernel Particle Method, are amenable to rigorous error analysis and preserve physical quantities (e.g., viscosity) by retaining the integral form, but have difficulties maintaining high-order numerical quadrature as particles advect. Given the promise of mesh-free methods to accurately model melting and relocation, the project will develop a novel mesh-free formulation with error estimation and validation incorporated from inception by resolving the key technological barriers impeding these methods: minimizing integration error as quadrature points move and resolving processes at the solid/liquid and liquid/air interfaces. To the best of our knowledge, these challenges remain unresolved in the literature and solutions are relevant to the nuclear weapons mission. Specifically, the former is necessary for solution verification while the latter is required to validate the complex physics. This project will provide a high-order quadrature mesh-free scheme implemented in a scalable software package. To understand interactions among all relevant processes, models for aluminum melting, oxidation, and flow will be included.

We are exploring mesh-free strategies for simulating metal melt and relocation that are currently unique at Sandia. Because particle methods can model large deformations and surface effects arising in many lab-relevant problems, this project has the potential for significant and broad impact.

## A PDE Constrained Optimization Approach for Crack Identification Based on Phase-Field Regularization

180879 | Year 2 of 2 | Principal Investigator: M. R. Tupek

### Project Purpose:

Computational simulations of engineering materials based on numerical solutions of systems of partial differential equations (PDEs) to determine the evolution of cracks and damage have been commonplace for decades. These forward problem approaches have proven utility in engineering design and analysis for many Sandia, NNSA, and DOE applications.

However, there are limitations to existing methodologies. One limitation is that commonly used models for predicting damage in materials are mathematically ill-posed. This results in simulation predictions which are highly sensitive to mesh and mesh resolution, making verifiable predictions difficult. In this project, we expand on recently proposed damage models that overcome this limitation and implement them in production codes developed at Sandia.

A second limitation is that predictions in and of themselves are not often the ultimate goal. More often the real objective of simulation codes is to use predictions to make decisions, improve designs, or determine physical conditions/parameters which led to observed results in the real world. In this work, we proposed and developed an unprecedented capability to solve highly nonlinear inverse problems involving fracture using partial differential equation (PDE) constrained optimization. Inverse problems solve optimization problems that are constrained by the relevant physics (elasticity, fracture mechanics, etc.), and are behind technologies such as topology optimization, parameter calibration, optimal control, automated design, etc.

There are several inverse problems involving fracture of interest to the engineering community, including: (1) nondestructive evaluation: determine existing cracks in a structure given observations of waves propagation; (2) crack forensics: determine what loads were applied to a structure that caused it to damage/fracture in an observed way; (3) nonlinear topology optimization: determine the optimal design of a structure to minimize the likelihood of crack propagation; and (4) heterogeneous material design: design the layout of a heterogeneous microstructure to maximize crack resistance. We focus on the last of these problems, but highlight that the techniques developed here are applicable to other highly nonlinear transient problems.



## Advanced Computational Methods for Thermal Radiative Heat Transfer

186367 | Year 2 of 2 | Principal Investigator: J. Tencer

### Project Purpose:

Assessing weapons safety in abnormal thermal environments using numerical modeling plays an extremely important role in assuring the safety of both the existing stockpile and ongoing life extension programs. Participating media radiation (PMR) is routinely neglected in full system simulations because, to date, it has been prohibitively computationally expensive. The methods investigated here have potential to reduce this computational resource constraint, improving simulation fidelity and increasing confidence in a number of high consequence applications of interest to the DOE (i.e., within the fire, weapon safety, and satellite communities).

In weapons safety assessments involving abnormal thermal environments, radiation heat transfer is frequently a dominant energy transfer mechanism. Radiation heat transfer can often dominate computational resource requirements (by several orders of magnitude) in these studies due to the nonlinear coupling between radiation and the other heat transfer modes and the dependence of the radiative intensity on direction. Presently, such analyses are impractical, even with current high performance computing resources. Consequently, analysts have often neglected participating media or have applied approximate models and other simplifications to reduce the computational expense to an acceptable level, at the expense of severely compromising the underlying physics. Organic encapsulants are widely used in weapon systems and they decompose at high temperature. This produces products that absorb, emit, and transmit significant thermal radiation.

The goal of this project is to make modeling of PMR tractable by applying more efficient computational methods. We will investigate novel approaches to improve the computational efficiency of PMR calculations, including data-driven reduced-order modeling approaches. This approach has been demonstrated to be applicable to one-, two- and three-dimensional radiation heat transfer problems with significant reductions in computational expense.

## Big Data Multi-Energy Iterative Volumetric Reconstruction Methods for As-Built Validation and Verification Applications

191069 | Year 1 of 3 | Principal Investigator: E. S. Jimenez, Jr.

### Project Purpose:

Identifying slight nuances of 'as-built' components is important in simulating dynamic systems such as explosive reactions. These systems are inherently chaotic; slight input deviations may create large changes in a given simulation. This problem is realized in the performance of idealized component models versus that of 'as-built' components. Strict tolerances are needed to ensure optimal performance; defects and imperfections cause degradation or failure. Sandia's computational tools, such as SIERRA and CTH, simulate these systems; however, inaccurate 3D experimental characterization introduces input errors that potentially generate significant computational errors.

Currently, 3D physical data generation uses computed-tomography (CT). CT is suboptimal in supporting segmentation of components with contrasting materials such as foam juxtaposed with metal due to artifacts and noise at the boundaries and interfaces. Instead, we propose a multi-energy iterative reconstruction (MEIR) method that produces superior volume reconstructions from x-ray images and improved materials identification through values proportional to elemental composition. The challenge in MEIR is the immense computational complexity (5th-order scaling in voxels). Furthermore, engineering datasets are six orders-of-magnitude larger than medical CT datasets, which is where current experience concentrates.

MEIR will fundamentally change experimentation and simulation validation at Sandia, enabling identification of defect influence in modeling. Improved ability to inspect, diagnose, and identify objects of interest directly leads to increased confidence levels of design, reliability, and assessment. Our goal is to produce substantially higher-quality images compared to traditional CT.

Big data MEIR has not been attempted due to risk related to the immense post-processing. The proposed novel acquisition technique explores nascent technology (with its own nontrivial risks) that potentially revolutionizes Sandia's advanced diagnostics and nondestructive testing (NDT) capabilities. If both succeed, then they transform NDT, big data science, advanced diagnostics, information management for engineering applications at Sandia, and Sandia's world-class radiography capabilities.



## Coarse-Grained Reactive Molecular Dynamics Simulations of Heterogeneities in Shocked Energetic Materials

191065 | Year 1 of 3 | Principal Investigator: A. P. Thompson

### Project Purpose:

Despite recent advances in our understanding of initiation of explosives, we are yet incapable of accurately predicting the shock to detonation transition in real nuclear weapon (NW) materials. The task is arduous; it spans many scales and involves diverse physical phenomena. It is well known that defects and discontinuities in the crystal structure play a key role in the onset of shock-induced chemical reactions and the ignition of hot spots. Using petascale computational resources to run massively parallel reactive molecular dynamics (RMD) simulations calibrated against quantum mechanical (QM) calculations, we are now able to directly simulate the initiation and growth of hot spots created at isolated heterogeneities of nanometer dimensions. However, a full description of initiation requires treating an interacting assembly of such heterogeneities, something that is beyond the scope of the RMD approach. Grain-scale continuum hydrodynamics simulations are now being used to describe the effect of shockwaves on representative assemblies of micron-size pores derived from experimental microstructures, but this approach is limited by the lack of validated materials models for submicron phenomena.

We propose to bridge between these two scales using a coarse-grained reactive molecular dynamics (CGRMD) approach based on dissipative particle dynamics (DPD). This will allow us to reproduce the temperature, stress, and extent of reaction fields obtained from RMD simulations of single heterogeneities, but at a fraction of the computational cost. The calibrated CGRMD model can then be scaled up to treat large assemblies of submicron heterogeneities that will be used to calibrate constitutive grain-scale models efficiently.

Existing programs support efforts to improve the fidelity of established methods at one particular scale. They do not support novel but unproven approaches for transferring knowledge between scales like that proposed here. This project will enable a completely new approach for modeling initiation in energetic materials.

## Developing Strong, Concurrent, Multiphysics, Multiscale Coupling to Understand the Impact of Microstructural Mechanisms on the Structural Scale

180877 | Year 2 of 3 | Principal Investigator: J. W. Foulk, III

### Project Purpose:

The mechanical performance of metallic structures is driven by microstructure. Strongly coupled processes can localize grain deformations through deformation twinning and void nucleation. We cannot observe, understand, or simulate the high-rate behavior of tantalum for the nuclear weapons complex or hydrogen embrittlement of austenitic stainless steels for gas transfer systems with phenomenology. Our ability to make engineering decisions hinges on our ability to resolve and couple microstructure.

The dominant dissipative mechanisms for candidate face-centered cubic (FCC) and body-centered cubic (BCC) metals result from intimately coupled processes evolving over many grains in the millimeter scale, embedded within a meter-scale structure subjected to abnormal or aging environments. We are required to invoke strong multiphysics and concurrent multiscale analyses to resolve failure processes. We are also required to move beyond crystal plasticity and develop discrete models for nanometer-scale deformation twinning and nanometer-scale void nucleation. The ability to enrich structural models with resolved microstructure creates a new computing paradigm that can only be realized with new computer architectures.

We propose to relate the inherent variability of microstructure to the performance of structures through significant contributions in coupling, adaptivity, grain-scale physics, and extensions to many core environments. We stress that these developments have general applicability to hierarchical systems (i.e., meter-scale) composed of many centimeter-scale components having millimeter design details with micrometer-scale defects that drive failure processes. The ability to assess system reliability through the resolution of flaws in forgings, cracks in glass, and debonding along interfaces will move Sandia from a reactive to a proactive approach for design, certification, and surveillance.

Solving multiple equations on multiple scales while adaptively propagating discrete deformation twins either directly or iteratively is an invasive computational proposition. This project enables the intense collaboration among material scientists, mechanicians, and computational scientists that will be required to span scales, physics, and architectures.



## Dynamic Mode Decomposition of Solids

193373 | Year 1 of 1 | Principal Investigator: C. Yarrington

### Project Purpose:

Dynamic mode decomposition (DMD) is a method that has gained notoriety in the field of turbulent fluid flows as a method for decomposing the flow field into modes that could be further deconstructed to understand their influence on the overall dynamics of the system. Forays into solids and nonlinear systems were considered, but not applied. In this work, DMD was applied for the first time to the heat diffusion and reactive heat diffusion equations on a random particle pack of uniform solid spheres. A verification of a linear heat diffusion test problem was successful, showing equality between the normal modes and Koopman modes obtained from DMD. Further application to a nonlinear reactive system revealed stability limits of the underlying modes which are dependent on microstructure and chemical kinetics. This work will enable the development of reactive material models based on further analysis using DMD to quantify the statistical dependencies of transient response on microstructural characteristics.

## Experiments and Computational Theory for Electrical Breakdown in Critical Components

173097 | Year 3 of 3 | Principal Investigator: F. J. Zutavern

### Project Purpose:

The phenomenon of electrical breakdown (EB) is a key issue for many electrical components, either the need to control it or prevent it entirely. For example, lightning arresters are designed to protect electrical systems by breaking down when struck by lightning. Alternatively, insulators in high energy density storage, switching, and transmission systems are designed to avoid breakdown. Predicting the performance and characteristics of these devices in extreme environments for stockpile and other critical applications is a key issue of national importance. For over a century, component designers have used the breakdown strength of bulk materials as a guide in many different environments, conditions, and configurations (that may have not been applicable/appropriate). Science-based modeling of EB has had limited success in predicting many of the observed characteristics, including location and size of primary current channels, damage on solid surfaces and in bulk insulating and multiphase materials, the generation and relative roles of ion and electron distributions in initiating and growing an electrical discharge, and the interaction with solid interfaces near breakdown events without the help of well-diagnosed and diagnosed discovery experiments.

This project will apply experimental diagnostics previously not applied to EB, such as ultra-short pulse laser terahertz imaging of electron distributions, that go beyond optical imaging to supplement the advancement of computational models. Discovery experiments and advanced diagnostics that provide insight into the spatial and temporal distributions of electron densities will be used to understand scientific issues, advance EB theory, and improve broad impact physics-based simulations.

Since technology depends on understanding EB phenomena, there is a strong demand for science-based predictive modeling that is presently limited to a few special cases. New experiments providing missing information represent a high risk which will benefit many areas of applied research and engineering critical to national interests.





## Experiments to Elucidate Fundamental Breakup Mechanisms of Molten Components in Shock Driven Flows

180876 | Year 2 of 3 | Principal Investigator: D. R. Guildenbecher

### Project Purpose:

High-speed, molten metal particulate is found in many applications of interest to Sandia, DOE, and other government agencies. Current predictive capabilities suffer from limited physical understanding of the complex interfacial phenomena associated with liquid metals. While significant knowledge exists on the interfacial instabilities which lead to the breakup of ordinary liquids, such as water, the breakup of liquid metals is much more complex due to substantially higher density and surface tension, oxide skins, potential phase change, and reactivity. New data and novel diagnostics are needed to understand these phenomena and derive next-generation models.

Towards this end, we will develop a unique experimental capability. Molten drops, generated using an innovative electrical heater design, will be subjected to shock-induced breakup in a shock tube. Quantitative measurements of the breakup process are made possible with Sandia's state-of-the-art digital in-line holography (DIH) capabilities. Previously, we have demonstrated DIH for 3D measurements of fragment sizes, velocities, and morphologies in low-speed flows. However, in this project, measurement uncertainty arising from thermal gradients, shock waves, and dense particulate clouds will challenge the DIH technique. To overcome this, we will combine nonlinear optical techniques, including phase conjugation and ballistic imaging, with the DIH diagnostic to yield revolutionary measurement capabilities. Successful development will allow for improved diagnostics of propellant fires, particle behavior in igniters, and additive manufacturing using molten metal sprays.

## Exploring the Influence of Microstructural Properties of Heterogeneous Explosives on Performance

180880 | Year 2 of 2 | Principal Investigator: T. Reedy

### Project Purpose:

Conventional detonators (exploding bridgewire and exploding foil initiators) rely on the bursting of an electrically conductive bridge element to deliver an impulse to the explosive which initiates detonation. However, the transfer of energy to the explosive and the physical processes which govern the initiation of chemical reactions and build-up to steady detonation within the explosive are not fully understood. The complicated physics of explosive initiation are assumed to include subsonic bed compaction, particle-to-particle interactions, development of hotspots, onset of chemical reactions, formation of a highly dense "plug" of explosive material, strong shock formation, and finally transition of the shock wave to detonation. It is postulated that these processes are linked to the internal microstructural properties of the heterogeneous explosive pellet. New diagnostic capabilities allow for the interrogation of the pellet's internal microstructure (such as local density and interface area), providing a more detailed and accurate description of the end-use form of the explosive than the loose, raw explosive powder. Moreover, CL-20 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane), the explosive to be examined within this investigation, is a new high-performance energetic material and has not been fully characterized in this manner. The aim of this project is to further the basic understanding and document the influence of the microstructural properties of heterogeneous explosives on performance. These performance data can be integrated into physically relevant grain-scale hydrocode models in the future, enabling the development of predictive capabilities for detonator performance.



## Exploring the Response of Jointed Structures to Blast Waves using a Shock Tube

193377 | Year 1 of 1 | Principal Investigator: J. Wagner

### Project Purpose:

A current limitation in blast-on-structure predictions at Sandia is our ability to model how energy is transferred from the blast field to jointed structures. Standard structural dynamics tests such as those using a shaker table are unable to replicate the loading environment associated with fluid dynamic flow fields and with blast waves. In this project, we address this shortcoming through a new joint experimental-computational approach. Jointed structures of interest are subjected to shock wave loading in Sandia's Multiphase Shock Tube. The main goal of this project is to investigate the feasibility of performing well-controlled experiments of fluid-structure interaction and blast-structure interaction environments in a shock tube. This represents the first attempt to look at nonlinear structural dynamics in a shock tube using advanced optical diagnostics.

## High Fidelity Coupling Methods for Blast Response on Thin Shell Structures

173095 | Year 3 of 3 | Principal Investigator: M. W. Heinstein

### Project Purpose:

Modeling a blast loading on thin shell structures, including initial structural failure and fragmentation through late-time over-pressure within the structure, is proving to be difficult. It is a multi-discipline problem involving a Lagrangian shell finite element description of the structure coupled with an Eulerian volume of fluid description of the air blast. Traditional approaches, including in-house solutions based on the Sandia codes CTH, ALEGRA, and Presto, have coupled Eulerian hydrocodes with Lagrangian structural dynamics codes using a staggered pressure-velocity mapping. Numerical experience has supported the theoretical view that such staggered coupling schemes can be numerically noisy and often unstable. Experience also shows that greater mesh resolution and pressure smoothing in the Eulerian domain can help but at great computational expense.

The research content in this project is the exploration of fluid-structure interaction methods to accurately capture the internal dynamic structural boundary condition in the Eulerian hydrodynamics and the conservative transfer of mass, momentum and energy constraints to the Lagrangian structural dynamics method. This project explored the question, "What could be a viable technology foundation for Sandia's next generation blast on structure modeling simulation capability?"

We demonstrated a credible, realizable coupling approach for shock loading of thin structures by *verifying the combination* of a fluid solver, structural solver and several potential coupling algorithms. Unique from previous work, we explored and verified coupling strategies and novel interface condition enforcement for large deformations. This work is relevant to the nuclear security mission, specifically safety and security assessments of nuclear weapons transportation systems.



## High-Density Signal Interface Electromagnetic Radiation Prediction for Electromagnetic Compatibility Evaluation

191072 | Year 1 of 3 | Principal Investigator: M. Halligan

### Project Purpose:

Quantifying the electromagnetic radiation properties of high-density interfaces is a significant challenge in the electromagnetic compatibility (EMC) design community. EMC engineers have struggled to assist designers in the development of these interfaces since robust, quantitative methods for comparing the radiated emissions of multiple designs have not been available. The scalability of high-density interfaces has compounded issues in developing characterization approaches since most analytical solutions are unique to specific geometries. We will pursue an analytical approach that can quantify the radiated power of high-density interfaces with few geometrical assumptions. Although the approach is shown to work well for small scale interfaces with fewer than ten signal lines at an interface, challenges remain in the developed approach in regards to its applicability to large interfaces with 10's or 100's of signal lines. A large amount of data is required to estimate the radiated power from large interfaces with the present theory, which may be impractical to acquire. The first objective of this project is to formulate a radiated power estimate from reduced data sets. Bounding approaches with the limited available data and applicable geometry symmetry at an interface may be used as the basis for the solution. The second objective of this project is to develop an approach to quantify the radiated power with practical, nonperiodic signal conditions which the present theory does not address. The solution for this objective will likely use statistical bounding methods to produce a statistical radiated power estimate.

## High-Throughput Material Characterization via 6-DoF Loading and Material Parameter Feedback Control using 304L SS as an Exemplar Material

191068 | Year 1 of 3 | Principal Investigator: P. L. Reu

### Project Purpose:

There is a general sense of disappointment about how well even our best numerical modeling tools performed in predicting material behavior and failure. An important reason for this poor performance is suspected to be inadequate material characterization. This could be due to inappropriate constitutive model form, incomplete material properties, or poorly calibrated material parameters. In the traditional characterization approach, the parameters of a given model are tuned to a simplified and limited set of experimental data (for example, uniaxial tension stress-strain curves). In many cases, this is insufficient information to adequately calibrate a sophisticated material model. Other loading modes are often desired (e.g., torsion, tension, impact, etc.), but the large number of tests required to characterize those modes is frequently sacrificed as a tradeoff to acquire a statistically significant number of tests for a single loading mode or parameter. This work will pursue the idea of multi-degree-of-freedom experimental load frame with complex specimen geometry designed using experimental simulations to optimize parameter measurement. Full-field data will be obtained using digital image correlation (DIC) tied to a multi-degree-of-freedom load frame (tensile, temperature, etc.) to create specific loading states to activate the various material parameters. We will study a complex and important nuclear weapon material, 304L, using these concepts. If successful, this capability will provide more complete material characterization with built-in uncertainty quantification (UQ), in fewer tests and at lower cost.

This ambitious project combines both simulation and experimental research beyond the superficial scale of validation experiments. This fundamental change in how Sandia treats model and experimental work will have applications well beyond material characterization and lead to improvements in both simulation uncertainty and experimental result interpretation.



## Magnetic Sensing to Determine Material Flows within Opaque Vessels

180875 | Year 2 of 3 | Principal Investigator: M. Nemer

### Project Purpose:

Many applications have a critical need for flow diagnostics that can be applied to high-temperature high-pressure (HTHP) opaque vessels and materials. Examples include liquefaction of organic materials (e.g., foam), potting of components with encapsulants, porous-media flows, thermal decomposition, and heat-exchanger optimization. Quantitative measurements of these phenomena within sealed vessels under HTHP conditions are particularly challenging, as optical access is often infeasible.

We are developing magnetic-field diagnostics to enable insight into flow in opaque vessels. This concept borrows ideas from both magnetic resonance imaging (MRI) and optical particle-imaging-velocimetry (PIV)/particle-tracking methods by seeding the fluid with magnetic dipole particles, applying time-varying fields to rotationally induce dipole alignment within well-defined regions, and then observing the flow-induced particle-driven time-varying magnetic field outside the vessel using small, low-cost, highly sensitive, commercially available magnetometers that are mass produced for consumer applications. The magnetic-field observations will subsequently be matched with numerical predictions through the application of efficient inversion techniques, and propagation of sensor and other sources of uncertainty through these inversion techniques.

Additionally, we are developing magnetic-field diagnostics to wirelessly measure temperature within opaque vessels. This method utilizes the temperature dependence of the magnetic field produced by permanent magnetic particles.

## Material Testing for Shear-Dominated Ductile Failure

189267 | Year 1 of 1 | Principal Investigator: E. Corona

### Project Purpose:

The representation of the behavior and failure of materials plays a very important role on the fidelity of computational models that Sandia uses to assess the strength and failure of structures subjected to severe loads. Many material models are available, and the choices that an analyst makes depend not only on the material and loading of interest, but also on how well and how easily the model can be calibrated. This project concentrates on developing specimens and methods to make the calibration process more complete and accessible. In particular, the focus was on failure under shear-dominated states, an area that has received little attention in the past, but also one that affects several important problems.

Four candidate specimen geometries and their associated quasi-static loading conditions were considered in this project with the objective of evaluating their suitability to generate ductile failure data when the state of stress was shear dominated. Two materials were considered for each geometry: an aluminum and a steel alloy. The aluminum alloy was significantly less ductile than the steel alloy. The intention was to see whether the same or different failure models would be required to fit failure data for different materials, especially those with significantly different ductility.





## Mechanics of Battery Degradation through Stress Driven Rearrangement of Percolated Conductive Networks during Discharge and Cycling

173098 | Year 3 of 3 | Principal Investigator: A. Grillet

### Project Purpose:

Mesoscale battery electrode structure and dynamics control electron and ion transport may determine capacity degradation in rechargeable batteries. This project will develop an understanding of the process of mechanical degradation on the electrode structure of lithium ion batteries, focusing specifically on the ionic and electronic percolation pathways. Building on research at the single particle level, we will examine how mechanical changes during cycling cause capacity fade through particle deformations and rearrangements, localized over-potentials, electronic isolation of particles, and lithium ion flux limitations. In particular, we will explore how structural heterogeneity coupled with anisotropic changes at the grain scale causes changes in the electronic conductivity of the percolated network. Understanding capacity fade and reliability of rechargeable batteries will have significant impact on our nation's ability to field advanced chemistries for electronics, munitions, and energy storage for renewable sources.

Whereas existing research on battery degradation has focused either at the battery level or on single particle changes, we will take a mesoscale approach, focusing on how microstructural behavior of the percolated electrode network drives macroscale battery performance. By coupling the complex network structure including structural heterogeneities, and correlated particle dynamics due to mechanical changes including anisotropic particle swelling and changes in modulus and porosity/tortuosity, the impact of cycling on battery performance can be understood. To date, this level of sophistication in developing coupled mechanics and performance models of the complex percolated structure of battery electrodes has not been developed, and represents a new way of looking at degradation mechanisms during cycling. This project will develop new experimental techniques to study battery electrodes examining the connectivity of both the particles and porosity as a function of both internal (lithiation) and external (applied) stresses. We will drive new methods of computationally coupling mechanics and electrochemical changes which will require development of anisotropic constitutive equations and composite network conductivity models to capture the progressive degradation.

## Modeling Primary Atomization of Liquid Fuels Using a Multiphase DNS/LES Approach

173096 | Year 3 of 3 | Principal Investigator: M. Arienti

### Project Purpose:

Atomization processes of injected liquid fuels determine the fuel-air mixture which subsequently controls combustion performance and emissions. Significant inadequacies in models that treat atomization are a major barrier to rapid development of high-efficiency, low-emissions combustion devices. While substantial improvements in the design of advanced devices are possible, even the most advanced experiments fail to provide information necessary to achieve this goal. High levels of precision are required that can only be reached through advanced simulation capabilities.

The main objective of this project was the coupling of realistic fuel spray injection dynamics with the large eddy simulation (LES) framework. The LES framework can treat the full range of multidimensional scales in turbulent reacting flows in a computationally feasible manner. Large energetic scales are resolved. Small subgrid scales are modeled. Thus, LES offers significant opportunities for predictive simulations in combustion devices for engineering applications. Modeling fuel atomization in the LES framework, however, posed several challenges due to the presence of the dynamically evolving interface boundaries of the injected fuel and subsequent dense spray.

A new framework describing the primary atomization of the fuel jet was developed through the extension of multiphase LES to dense sprays with the support of a database obtained from model-free, direct numerical simulations (DNS) of fuel injection. Both multiphase LES and DNS computer codes are unique to Sandia. This new LES model was embedded in the existing combustion LES framework to provide an advanced multiscale closure for predictive simulations of fuel distribution from injection to combustion. Because of highly nonlinear physics involved, the development of a viable multiscale closure for predictive simulations of primary liquid atomization required: 1) an innovative mathematical representation of dense sprays consistent with the existing large eddy simulation framework and 2) computationally intensive benchmark cases, carried out on much longer time frames, thanks to Sandia's computational facilities.



## Multiscale Now! A Novel Hierarchical Approach for Multiscale Structural Reliability Predictions of Ultra-High Consequence Systems

180878 | Year 2 of 3 | Principal Investigator: J. M. Emery

### Project Purpose:

This project will impact Sandia's safety mission through development of robust yet tractable multiscale structural reliability capabilities for uncertainty quantification (UQ). We do not focus on creation of a multiscale numerical method (MNM), but, rather, on *innovative tools* that uniquely combine Sandia's current investments in MNMs for multiscale UQ. Prediction of structural failure due to strain localization or fracture is essential to Sandia's safety mission where ultra-high reliability (e.g., failure probability  $<1e-06$ ) is required. Heterogeneity at the fine scale contributes to significant uncertainties in performance. Due to the exorbitant computational demand, engineering applications cannot include fine-scale details throughout the problem domain, and brute force Monte Carlo simulation (MCS) is impractical. A concurrent MNM is necessary but not sufficient.

We will develop a novel hierarchical solution that will: 1) systematically focus computational resources at requisite hotspots through a hierarchy of analyses, 2) combine analyses of variable fidelity to maximize efficiency, 3) make MCS tractable using stochastic reduced-order models (SROMs), and 4) be validated with a first-of-its-kind multiscale experimental technique.

This project advances a new concept for multiscale structural reliability prediction and will provide proof-of-principle application to ductile alloys. It uses an innovative hierarchical scheme that combines predictions of varying fidelity to compute the probability of failure of a component. There are significant risks, but if successful it will benefit a broad range of structural reliability applications.

## Novel Method to Characterize and Model the Multiaxial Constitutive and Damage Response of Energetic Materials

180883 | Year 2 of 3 | Principal Investigator: M. J. Kaneshige

### Project Purpose:

This project aims to create a scientific breakthrough in the ability to predict the mechanical behavior of energetic materials through the design of a new multiaxial testing method using 3D digital image correlation (DIC) and the development of a novel continuum damage mechanics (CDM) based constitutive model for the volumetric and deviatoric response of energetic materials. Traditional methods to elucidate the volumetric and deviatoric response of energetic materials require the use of complex load frame configurations, which apply hydrostatic pressure and uniaxial loads independently. This new method will utilize a variation of the Bridgman notched specimen method and through 3D optical strain measurements elucidate the multiaxial constitutive and damage behavior through comparison to the analytical (skeletal stress) or elastic finite element (FE) solution. This work will be extended to deal with effects of strain rate ( $0.001$  to  $1\text{ s}^{-1}$ ) and temperature (ambient to  $75\text{ }^{\circ}\text{C}$ ). The primary challenge of this effort is transforming the Bridgman method that was originally developed for metals under tension towards energetic materials under compression. An outcome of this novel characterization method is the development of a CDM-based constitutive model for the prediction of the "batch-to-batch" mechanical behavior of energetic materials. This model will be used to simulate the service conditions of mock plastic bonded explosive (PBX) material including uniaxial and multiaxial states of static and dynamic loading. This work is in collaboration with the University of Texas at El Paso.

Mechanical response of energetic materials has cross-cutting impact on diverse programs and problems. Structural material models are often adapted but are generally inadequate. Understanding the mechanical response of energetic materials is necessary for science-based assessment and assurance of the reliability of penetrating weapons and the safety of weapons subjected to abnormal thermal, mechanical, and combined environments. The experimental and modeling tools developed under this project will address significant gaps in engineering models used to answer critical national security questions.



## Plasma Tailoring Technology

193376 | Year 1 of 1 | Principal Investigator: R. F. Hess

### Project Purpose:

This project was focused on understanding the manufacturing challenges associated with producing doped composite materials and simulating their effect on plasma generation. Theoretical studies dating back to the 1950s suggest the possibility of creating a layer of charged particles around an aerospace vehicle to reduce friction by injecting momentum energy into the boundary layer. This theoretical work has focused on coatings that would either ablate too quickly or be so heavy that they would alter flight dynamics. This project focused on answering significant material science challenges (experimental and theoretical) to verify the hypothesis that the addition of electron emitting dopants to composites can adjust plasma characteristics without compromising the overall aerospace system operational characteristics. Past studies were only theoretical in nature and this project differs from previous work in that it was a closely coupled manufacturing-testing-simulation effort. We produced a series of unloaded and dopant loaded phenolic coupons and tested their ablation performance in the Solar Furnace. A parallel modeling effort using PIRATE was also conducted to investigate electron density effects in the boundary layer.

## Process Modeling for Additive Manufacturing

180881 | Year 2 of 2 | Principal Investigator: L. L. Beghini

### Project Purpose:

Additive manufacturing (AM) provides a new avenue to design innovative materials and components that cannot be created using traditional machining operations. With current AM capabilities, complex designs (such as those required in weapon systems) can be readily manufactured with laser powder forming (or Laser-Engineered Net Shaping (LENSTM)) that would be otherwise cost prohibitive or impossible to produce. However, before an AM product can be qualified for weapon applications, the characteristics of the metals produced by additive manufacturing processes need to be well understood. This project investigated the development of computational simulation tools to model metal additive manufacturing processes by further extending and integrating existing Sandia tools to accomplish the following:

- Be able to predict residual stresses in AM product
- Extend high-fidelity material models to capture material evolution during the formation process, leading to prediction of end-state material properties
- Provide a basis for engineering tools to propose improvements to additive manufacturing process variables, including those that minimize process variation

This project developed a new modeling tool/capability, which had not been previously attempted nor documented in the literature. While this work is directly applicable to additive manufacturing processes, the tools developed have potential to help enable modeling welding processes such as gas tungsten arc (GTA), electron beam, and laser welding.



## Reduced Order Models of Structures Incorporating Complex Materials

191074 | Year 1 of 3 | Principal Investigator: R. J. Kuether

### Project Purpose:

We plan to develop a reduced order model (ROM) capability that will be the first to incorporate nonlinear and time-dependent material behavior, which will significantly improve the computational efficiency and accuracy of large, component-level simulations of dynamic loading events. While predictive finite element (FE) models have been developed to supplement or replace physical experiments, they require millions of degrees-of-freedom (DOFs) and intricate constitutive models that demand enormous computational resources. Our proposed ROM technique will greatly reduce the burden associated with simulating full order FE models of a variety of nuclear weapon (NW) components.

Current ROM techniques, such as the Craig-Bampton method, are used with *linear elastic* FE models, but they cannot incorporate the important nonlinear and time-dependent material behavior exhibited by many NW materials (e.g., foams, rubbers, composites). To overcome this severe limitation, our primary technical challenge is to develop a ROM in parametric form using a physics-based approach. We will address this challenge by adapting state-of-the-art model reduction techniques for certain types of nonlinearity (large deformations and contact) to describe the material behavior of interest. If successful, this research will: 1) facilitate development of accurate and computationally efficient predictive models that simulate dynamic behavior of component-level structures, 2) enable uncertainty quantification and optimization analyses of the model, and 3) enable analysts from multiple organizations to share structural dynamics models without requiring access to the native FE software.

Our project requires significant theoretical development and verification before it can draw interest from mission initiatives. Successful completion of this project will have a large and broad impact on critical mission areas, such as quantifying component-level design boundaries for hostile dynamic load environments.

## Reducing the Adverse Effects of Boundary-Layer Transition on High-Speed Flight Vehicles

173878 | Year 3 of 3 | Principal Investigator: K. M. Casper

### Project Purpose:

During boundary layer transition, high pressure fluctuations are generated on a reentry vehicle that can create significant vibration of internal components. There is an ongoing effort at Sandia to better predict these fluctuations and also understand how they couple to the vibration of the structure. Modern computational capabilities now allow modeling of the fluid-structure interactions in these hypersonic vehicles. These models must be developed from experimental data; however, current structural testing of hypersonic vehicles relies on static tests that do not provide an accurate representation of the fluid-forcing environment in flight. We will make novel measurements of this coupling by introducing controlled pressure disturbances over a flexible panel in hypersonic flow. The flow field and panel response will be characterized using high-frequency pressure and vibration measurements as well as flow-field visualization. High temporal resolution is required to resolve the unsteady flow field at hypersonic speeds, but these diagnostics have only recently attained the frequency response necessary to study this problem.

The project seeks to generate a unique hypersonic dataset to provide physical understanding of how transitional pressure loading creates an elevated structural response. This work has never been attempted because of its complexity: the design of the model, flow perturber, and thin panel all require significant research and risk in their development. The subsequent experiments and data analysis will require substantial time, effort, and future development before the fluid-structure interactions can be well understood. The enhanced capabilities could be utilized in the future for hypersonic projects relevant to DoD and NNSA national security missions.





## Shock Capability Development for Flight Simulation Inertial Testing

193375 | Year 1 of 1 | Principal Investigator: R. A. Jepsen

### Project Purpose:

Compelling evidence supporting the importance of combined environments in testing suggests that other known environments in flight should also be developed such that they can be combined with the inertial loads from centrifuge testing. The addition of vibration with inertial loads (Vibrafuge) has been developed and studied extensively. The addition of spin with vibration and inertial loads is also being developed (Superfuge). An important aspect of flight environments yet to be combined includes staging and separation shocks that occur during flight. Inclusion of these environments will further Sandia's commitment to testing systems to the most realistic environments possible while strengthening the confidence and reliability of our systems.

## Turbulent Flow UQ using Machine Learning Techniques

191076 | Year 1 of 3 | Principal Investigator: M. F. Barone

### Project Purpose:

Modeling fluid structure Interaction (FSI) is a key element in defining random vibration environments for weapons in captive carriage and reentry systems, and for predicting the dynamics of wind turbine structures. Successful modeling of FSI requires accurate prediction of the turbulence-induced loads on the structure. Typical simulation methods, such as Large/Detached Eddy Simulations (LES/DES), suffer from uncertain and often large errors due to turbulence modeling. This yields predictions of pressures (loads) and responses with inconsistent accuracy and large uncertainties. Physically, these loads are generated through highly nonlinear and nonlocal mechanisms, and hence, the origins of errors in their predictions are poorly understood. This problem pervades all nonlinear modeling applications – use of models based on ad hoc phenomenological arguments results in large, poorly understood uncertainties, compromising reliability of the predictive simulations. In the fluids domain, model-free direct numerical simulations (DNS) are increasingly feasible on current platforms and can be used to quantify these origins and sensitivities. However, extracting sensitivity information from the massive amounts of data generated by these simulations is an enormous challenge. Machine learning (ML) methods, specifically designed to work with large amounts of data and extract such dependencies have the potential to transform our ability to quantify and address these uncertainties.

In this project, we will develop ML methods to quantify sensitivities and uncertainties in predictive engineering simulations. We focus on FSI problems and target the development of ML-based methods to characterize and quantify uncertainties in predicted loads due to turbulence modeling using data from DNS. Success here can alter the paradigm for model development, improving reliability of predictive simulations.



## Understanding Hot Spot Initiation using Electronic Ultrafast Sum Frequency Spectroscopy

180874 | Year 2 of 3 | Principal Investigator: J. J. Kay

### Project Purpose:

Although shock initiation of explosives has been studied for decades, it is still not clear how shock waves initiate chemical reactions that lead to detonation. Understanding the sequence of reactions involved in initiation is critical to predictive understanding of energetic material performance. At present, we have little predictive understanding of the shock sensitivity of energetic materials, and therefore, limited capacity to predict initiation thresholds and uncertainties in explosive components.

“Hot spot” initiation is one key aspect of the problem that remains unanswered. It is empirically well-known that material porosity enhances shock sensitivity, and it is often assumed that localized heating initiates reactions at defect sites. However, a wealth of evidence indicates that the mechanism may not be thermal heating, but rather spontaneous pressure-induced decomposition. This alternate mechanism is postulated to involve shock-induced changes in the electronic structure of the material, in which instantaneous reactions occur at the shock front, assisted by local distortion of electronic structure at defect sites. At present, no definitive measurement or calculation has proven or disproven this mechanism.

In this project, we are investigating this energy localization mechanism in explosives using ultrafast spectroscopy. We are performing a series of spectroscopic measurements to determine whether this pressure-induced reaction mechanism can properly explain hot spot initiation. These measurements will answer, once and for all, whether pressure-induced reactions are important in shock initiation. Answering this pivotal question will assist predictive modeling of shock initiation in energetic materials, which ultimately assists development and certification of explosive components at Sandia.

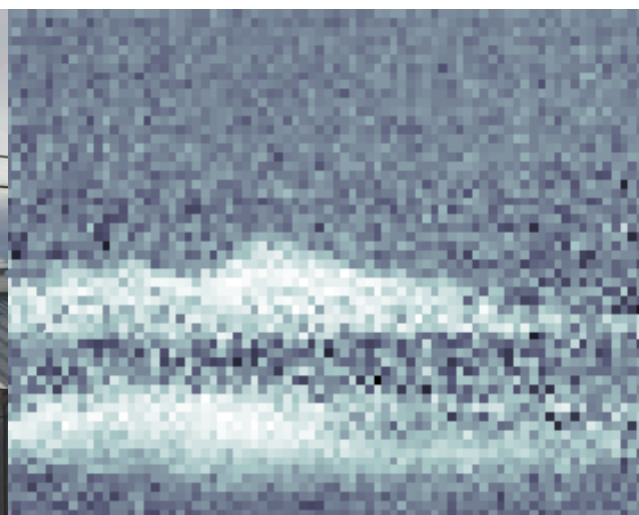
## Understanding Soot Development and Thermal Stratification in Combustion Engines through Hyperspectral Non-linear Optical Diagnostics

191060 | Year 1 of 3 | Principal Investigator: C. J. Klierer

### Project Purpose:

New emissions regulations in the US and abroad require reductions in the quantity of soot and  $\text{NO}_x$  emitted from heavy-duty diesel engines to alleviate both environmental and health concerns. Several improvements are being developed in diesel engines to meet these new requirements, including both exhaust after-treatments and in-cylinder combustion modifications. While several in-cylinder strategies are currently being pursued, the mechanisms by which soot reduction is achieved are still widely debated. Much lower (near-zero) particulate and  $\text{NO}_x$  emissions can be realized in homogenous charge compression ignition engines (HCCI), but the maximum load for a given intake pressure is often limited by an overly rapid combustion-induced pressure rise, which limits the ability to operate over the required range of loads and speeds. However, recent observations of thermal stratification in HCCI engines suggest a possible path to more widespread feasibility. In order to optimize engines with decreased in-cylinder soot production and  $\text{NO}_x$  emissions, a fundamental understanding of soot formation and oxidation rates, as well as the thermal stratification formed during the HCCI compression stroke is required. Therefore, we propose to develop coherent Raman optical diagnostics, which will enable the in situ measurement and imaging of the instantaneous thermal field, and the relative concentrations of  $\text{O}_2$ ,  $\text{H}_2$ , and  $\text{N}_2$ , in optical engines with significantly higher accuracy than ever before achieved. The diagnostics cultivated here will mitigate the effects of scattering, beam-steering and high-pressure spectroscopic interferences and will provide an ultimate canonical data set needed for experimental validation and feedback to engine simulation codes.

Optical measurements in combustion engines are extraordinarily difficult, due to conditions that yield most optical techniques impractical for use. Ultrafast coherent Raman imaging holds promise for high fidelity measurements of key scalars in engines. While high risk, successful completion of the project will have significant impact in engine research.



## Geoscience

The Geoscience Investment Area seeks to expand the frontiers of knowledge in the following areas: 1) the properties, structure, phenomena and processes associated with the earth's subsurface, surface, and atmosphere and 2) how engineered systems interact with the earth and the earth system. These earth systems and properties impact Sandia national security missions, including energy security, defense, nonproliferation, disaster response, and climate security.

*The images above show: (left) photo of a mountain being imaged (right) from horizontally traveling muons (subatomic particles) in telescopic mode. The lighter area in the top portion of the figure on the right represents the mountain in the photo on the left. The lighter area in the bottom portion of the figure on the right is due to "noise" from muons detected from the opposite direction. (Project 173101, Imaging the Subsurface with Upgoing Muons)*

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## Chemical-Mechanical Modeling of Subcritical-to-Critical Fracture in Geomaterials

191133 | Year 1 of 3 | Principal Investigator: L. Criscenti

### Project Purpose:

Predicting fracture initiation and propagation in low-permeability geomaterials is a critical, yet unsolved problem, crucial to assessing shale caprocks at CO<sub>2</sub> sequestration sites, and maximizing/controlling fracturing for gas and oil extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material and altering crack nucleation and growth rates. However, engineering the subsurface fracture environment has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables.

We will develop a fundamental atomistic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations to produce characteristic continuum-scale metrics for comparison with experiments. The connection to the macroscale will involve development of chemical-mechanical fracture theory, novel estimators of chemical forces acting on the crack, and the never-before application of this theory at the atomic scale. Although we target geomaterials, this capability can have direct impact on predicting the corrosion and embrittlement of metals and ceramics. Strategically, this project will make Sandia a leader in coupling mechanical and chemical controls in geoscience applications and fill a critical gap in interpreting experimental results. Elucidating the chemical mechanisms that promote fracture will guide the choice of fracking fluids and result in cost efficiencies, a reduction in water usage, and more environmentally benign chemical selections.

This effort has the potential to make revolutionary contributions to the technical factors that control subsurface fracture by coupling chemical and mechanical mechanisms, specifically at the atomic scale—a completely new application in fracture theory. The work will also provide modeling capabilities that treat relevant aspects of the complex subsurface environment plus vital understanding of the dominant mechanisms.

## Detection of Soluble Ligand-Tuned Molecular Tags for Subterranean Fluid Flow Monitoring Using Resonance Raman Spectroscopy

191085 | Year 1 of 2 | Principal Investigator: R. Kemp

### Project Purpose:

Monitoring underground reservoir flows is critical to efficient geothermal/hydrocarbon energy recovery. Approaches to solve this issue can involve loading “trackable” materials (tags) into porous proppants used in the energy recovery process, and then following these materials as they diffuse into the hydrocarbon/water streams. Detailed analytical identification of the tag aboveground can give production engineers valuable information about both the location and the flow rates of the product streams. Ideally, a large number of tags would be loaded underground, thus allowing a more precise mapping of the reservoir to be accomplished. In order to accomplish this goal, we will develop tags that must be uniquely identifiable and stable within the system. Additionally, tags that can be gradually released over time allow for many months of observation to occur, thus enabling the engineers to focus on product producing zones.

Our novel approach involves a molecular ligand-based system that allows the facile syntheses of >>100 base-metal complexes containing modified multidentate porphyrins, phthalocyanines, or related Salen ligands. We will demonstrate an enhanced sensitivity of these complexes to detection by resonance Raman spectroscopy (rR). These molecular complexes can be easily designed to allow solubilities of ~100% water to ~100% hydrocarbon, and importantly are virtually unlimited in the number of possible candidates. These highly stable complexes mimic compounds found naturally underground, but are easily distinguishable using rR.

Along with experiments, molecular dynamic simulations will be conducted to evaluate the adsorption and diffusion of representative moieties with natural surfaces to provide atomistic insight at the interface. Modeling results will be fed back into the experimental synthetic program to provide guidance on ligand modifications that will create new signaling agents for use in both hydrocarbon and water systems.





## Developing Fugitive Emissions Sensor Networks: New Optimization Algorithms for Monitoring, Measurement and Verification

193231 | Year 1 of 3 | Principal Investigator: K. A. Klise

### Project Purpose:

The oil and natural gas industry relies on a complex network of infrastructure for production, processing, transmission, and storage. This infrastructure is subject to routine emissions that are part of normal operations. Normal emission rates can vary greatly. Furthermore, individual sites are subject to complex wind patterns that transport emissions to surrounding regions. Within this framework, it is important to quickly detect operational upsets to ensure emission levels are within scope.

Continuous or regularly scheduled monitoring has the potential to quickly identify changes in emissions. However, even with low-cost sensors, only a limited number of sensors can be placed in the field. The physical placement of these sensors and the sensor technology used can have a large impact on the performance of a monitoring strategy. Furthermore, sensors can be placed for different objectives, including maximum coverage, probability of detection, or to quantify emissions. Different monitoring objectives may require different monitoring strategies, which need to be evaluated by stakeholders before sensors are placed in the field.

In this research, we are developing optimization software to enhance detection programs through optimal design of the monitoring strategy. These methods integrate atmospheric transport models with sensor characteristics, including fixed and mobile sensors, sensor cost and failure rate. The methods use site specific conditions which capture differences in meteorology, terrain, concentration averaging times, gas concentration, and emission characteristics. Mixed-integer, stochastic programming is used to solve for sensor locations and sensor type that maximize the effectiveness of the detection program.

## Development of a Downhole Technique for Measuring Enthalpy in Geothermal Reservoirs

191092 | Year 1 of 2 | Principal Investigator: G. Cieslewski

### Project Purpose:

The amount of thermal energy (enthalpy) contained in geothermal fluid is one of the key parameters used to determine the value of a geothermal resource and is vital for understanding the performance of existing reservoirs. The enthalpy of a single-phase fluid can be determined from the temperature and pressure of the fluid; however, as hydrostatic pressure decreases, geothermal fluids often become two-phased and enthalpy calculations require knowledge of the steam and water fractions. Current surface-based methods for measuring enthalpy are expensive and complicated, providing an incomplete view of downhole enthalpy. Downhole measurement of enthalpy would enhance understanding of geothermal resources and allow for improved measurement of energy produced from different fracture zones.

We will develop a method and apparatus for measuring the downhole enthalpy of a flowing geothermal fluid in real time at high temperature (HT) and pressure. Our method involves measuring the concentration of select naturally occurring ions found in the liquid phase of the geothermal fluid throughout the wellbore. The change in liquid-phase ion concentration will be used to calculate the proportion of liquid to steam which can be combined with temperature and pressure measurements to enable measurement of enthalpy. While benchtop instrumentation exists for routinely measuring ion concentration under ambient conditions, the sensing materials and supporting electronic components in these devices are unable to survive in harsh geothermal environments. While the primary impetus of the design is for geothermal resources exploration, the proposed sensor could be used for real-time monitoring of coolant quality in nuclear reactors.

This research will allow for previously unattainable real-time chemical and thermodynamic measurements in harsh environments. Developing chemical sensors that are capable of surviving these harsh environments carries with it a number of high risks including ensuring the ion selective membrane is stable in hot corrosive brine while maintaining a high degree of selectivity for the target ion.



## Digital Rock Physics for Multi-Scale Experiments and Modeling of Fractured Porous Media

191129 | Year 1 of 2 | Principal Investigator: M. J. Martinez

### Project Purpose:

About 80% of US energy currently comes from subsurface sources. Subsurface strata are ubiquitously fractured at nearly every length of geotechnical interest. Understanding and control of subsurface fractures and fluid flow is key to development of a secure energy future. Today, we cannot accurately image, predict, or control fractures with confidence or in real time. Mesoscale analysis—linking discrete and complex pore-scale behavior to macroscale reservoir response—remains elusive as a result of the extreme heterogeneity and resulting scale dependence of porophysics, but is required for a generalized understanding of fractured porous geomaterial behavior during subsurface engineering.

We apply recent advances in 3D printing technology with a 3D digital rock approach to examine behavior of reproducible fractured porous structures derived from x-ray computed microtomography (micro-CT) imaging of real fractured rocks. An ambitious schedule of experiments and mesoscale modeling will elucidate the poromechanical relation between solid stress and pore pressure on flow path topology and fracture permeability. The use of 3D printed microstructure allows us to surmount problems associated with sample-to-sample heterogeneity that plague rock physics testing and, therefore, test material response independent from pore-structure variability. This project is a testbed to develop the methodology for use of additively manufactured copies of real rock in lab testing, which is a potentially disruptive technology for geosciences, engendering all manner of possible experiments on reproducible specimens. The outcome will advance constitutive models for flow in fractures, effective stress, fracture closure and permeability that directly impact our ability to predict subsurface operations in fractured rock.

## Fundamental Study of Disposition and Release of Methane in a Shale Gas Reservoir

173102 | Year 3 of 3 | Principal Investigator: Y. Wang

### Project Purpose:

The boom in shale gas production through hydrofracturing may reshape the energy production landscape in the US. However, one troubling issue related to shale gas extraction is the decline in wellbore production by up to 95% over the first three years, with a recovery rate less than 10%. Maximizing wellbore production and extending the production lifecycle are crucial to realize the energy security benefits of shale gas. This effort has been hindered by a lack of mechanistic understanding of gas disposition and release in shale gas reservoirs. Existing knowledge drawn from conventional gas-oil reservoirs is not applicable to shale formations characterized by nanometer-scale pore sizes and extremely low permeability. Gas in shale (mainly methane) exists as a compressed gaseous phase or an adsorbed phase in nanopores, with the latter accounting for up to 85% of total gas in place (GIP). We will perform an integrated experimental and modeling study to fundamentally understand two important processes that directly control GIP in a reservoir and wellbore production: methane partitioning in the nanopores of mudstone matrices, and methane transport from low-permeability matrices to fractures. We will first carefully characterize pore geometry and pore-size distributions of representative shale samples. We will then measure methane sorption isotherms, desorption kinetics, and transport properties on selected shale samples, either crushed or intact, under simulated reservoir conditions, using our newly developed high temperature/high pressure (HTHP) systems and microanalysis techniques. The data will be synthesized, using novel nanogeochemistry and nanofluidics concepts and molecular dynamic simulations to establish needed constitutive relationships for predicting and optimizing shale gas wellbore production. The project will leverage Sandia's unique expertise in material science, nanogeochemistry, HTHP geochemistry, and high performance computation capability. If successful, this work will advance research of shale gas, particularly in areas related to nanogeochemistry, as well as prediction of material behaviors in extreme environments, greatly impacting DOE's energy security mission.



## Geomechanics of Induced Seismicity in CO<sub>2</sub> Reservoirs

193418 | Year 1 of 2 | Principal Investigator: P. Newell

### Project Purpose:

Injection of wastewater, including formation water coproduced with oil and gas from hydrocarbon reservoirs, is routinely practiced on a large commercial scale. In some occurrences, increased rates of seismic activity are reported in the vicinity of injection wells and attributed to fluid injection. While the fundamental geomechanical processes linking fluid injection and seismic fault slip are well known and documented, the correlation between injection activity and seismic events is, in many cases, based on their spatial and temporal association, some with a pore-pressure disturbance analysis but without a site-specific geomechanical analysis.

This project assesses the effects of fluid injection into porous sedimentary formations on the stability of nearby faults extending into crystalline basement using coupled (thermo-) poroelastic numerical simulations with boundary conditions applicable to the industrial scale injection of wastewater and anthropogenic CO<sub>2</sub>. Using 3D finite element simulations, we assess the effects of the poroelastic and thermo-poroelastic response in pore pressure in the reservoir and in overlying and underlying units and the resultant change in Coulomb shear stress on nearby faults.

## High Fidelity Hybrid Method for In Situ Borehole Stress Determination

191087 | Year 1 of 3 | Principal Investigator: M. D. Ingraham

### Project Purpose:

The in situ state of stress affects every activity in the subsurface, from mining and resource extraction to waste storage in the form of deep borehole or mined reservoirs. Although a variety of methods exist for “measuring” in situ stress, the dominant means are borehole methods wherein hydraulic fractures are induced or breakouts are examined across a wellbore interval. Errors in magnitude and orientation from these methods can be as high as 30 to 40% (JASON, 2014) and result from rock heterogeneity, anisotropy, and uncertainty in the physics of rock failure. This is especially true in: 1) high-temperature high-pressure geothermal applications in rocks, such as granites and 2) in anisotropic and heterogeneous shale formations for oil, gas, and carbon storage.

The intent of this project is to explore these two arenas through a combination of laboratory experiments (some of which are performed in conjunction with the University of Wisconsin), advanced rock mechanics theory, numerical modeling, and investigating historical borehole measurements to develop a hybrid method of borehole stress determination along with a set of “best practices” guidelines for quality assurance in interpreting wellbore stress data. This project will result in new knowledge of the interdependence of mechanical, chemical, and thermal effects on rock properties and an improved understanding of borehole breakout and hydraulic fracture. The results will improve the understanding of borehole data and lessen the error bounds on historical measurements.

This work stands apart through the combination of true triaxial test results with modeling of borehole breakouts. Previously, there have been publications on breakouts in pre-stressed rock that has been drilled, but not coupled with modeling of the breakouts, and coupling the modeling, properly parameterized with laboratory data, with an examination of historical data will provide new and insightful results that will help reduce the uncertainty of in situ measurements.



## Imaging the Subsurface with Upgoing Muons

173101 | Year 3 of 3 | Principal Investigator: N. Bonal

### Project Purpose:

The purpose of this project is to develop subsurface imaging using muons. Subsurface imaging of underground structures, such as tunnels and caverns, is important to Sandia's missions of energy surety, nonproliferation, and border and infrastructure security. Muons are subatomic particles produced in the upper atmosphere, which penetrate the earth's crust up to few kilometers. Their absorption rate depends on the density of the materials including fluids through which they pass. Measurements of muon flux rate at differing directions provide density variations of the materials between the sky and detector from those directions, much like a CAT scan. Traditional muon imaging focuses on more prevalent downgoing muons, but requires below-target detectors—a major obstacle to widespread use. This work consists of three parts: 1) assess the use of muon scattering for estimating density differences of common rock types, 2) detect a void in a large volume of rock using muon flux, and 3) measure muon direction to differentiate upgoing from downgoing muons by designing a new detector.

## Monitoring, Understanding, and Predicting the Growth of Methane Emissions in the Arctic

173100 | Year 3 of 3 | Principal Investigator: H. A. Michelsen

### Project Purpose:

Concern over Arctic methane ( $\text{CH}_4$ ) emissions has increased following recent discoveries of poorly understood sources and predictions that methane emissions from known sources will grow as Arctic temperatures increase. Methane has a 25-fold higher global warming potential than carbon dioxide ( $\text{CO}_2$ ) and is believed to cause ~50% of the net radiative forcing of  $\text{CO}_2$ . The calculated capacity of the warming Arctic to produce methane is enormous, and the warming effect of  $\text{CH}_4$  could surpass that of  $\text{CO}_2$ . Methane sources predicted to increase include: thawing terrestrial permafrost, shallow oceanic methane hydrates, and submerged permafrost. Recent studies revealed an unexplained methane source associated with cracks in sea ice and a potentially important open-ocean source. A few incomplete datasets are available to study Arctic methane emissions, and new efforts are required to detect increases and explain sources without being confounded by the multiple sources. Methods for distinguishing different sources are critical. We are conducting measurements of atmospheric methane and source tracers and are coupling these measurements with global atmospheric modeling and back-trajectory analysis to identify, characterize, and assess the climate impact of Arctic methane sources. The unique data and analysis addresses a timely and high profile scientific question. Understanding Arctic methane sources will help inform decisions related to human activity (such as oil and gas exploration) at high latitudes.

The goal of this project was to address uncertainties in Arctic methane sources and their potential impact on climate by: 1) deploying newly developed trace-gas analyzers for measurements of methane, methane isotopologues, ethane, and other tracers of methane sources in Barrow, AK, 2) characterizing methane sources using high-resolution atmospheric chemical transport models and tracer measurements, and 3) modeling Arctic climate using the state-of-the-art, high-resolution Spectral Element Community Atmosphere Model (CAM-SE) developed at Sandia.





## Real Time Degassing of Rock during Deformation

191137 | Year 1 of 2 | Principal Investigator: S. J. Bauer

### Project Purpose:

Noble gases emitted during natural and man-made rock deformation could be used to sense changes in the stress state and deformation, for instance, earthquake prediction and subsurface detonation detection. When rock is subjected to stress conditions exceeding about half its strength, it begins to crack. With increasing differential stress, cracks coalesce into a macrofracture. Newly formed cracks, inter and intragranular rock surfaces release accumulated radiogenic and nucleogenic noble gases contained within minerals (e.g.,  $^4\text{He}$ ,  $^{21}\text{Ne}$ , and  $^{40}\text{Ar}$ ). Fracture network evolution changes the material's transport properties, and affects radiogenic gas migration within the underground system to the sampling point. Thus, changes in gas emanation from rocks could be used to infer changes in stress state and deformation. The gas composition emitted depends on lithology, geologic history and age of the rock, fluids present, and uranium, thorium and potassium-40 concentrations in the rocks that affect the production of radiogenic noble gases. The composition of emanated gases during deformation progresses and should inform us on stress/strain state changes in subsurface systems. For the first time, we will collect real-time gas samples during deformation with acoustic emissions and volume strain, leveraging Sandia's unique capability of rare gas analysis and rock deformation. These gases could be tracers of subsurface deformation providing potential signals for evaluating changes in crustal stress state, earthquake prediction, volcanic monitoring, and stress/strain detection in underground detonations and excavations.

## Self-Tuning Seismic Sensor Data Processing

180882 | Year 2 of 3 | Principal Investigator: T. J. Draelos

### Project Purpose:

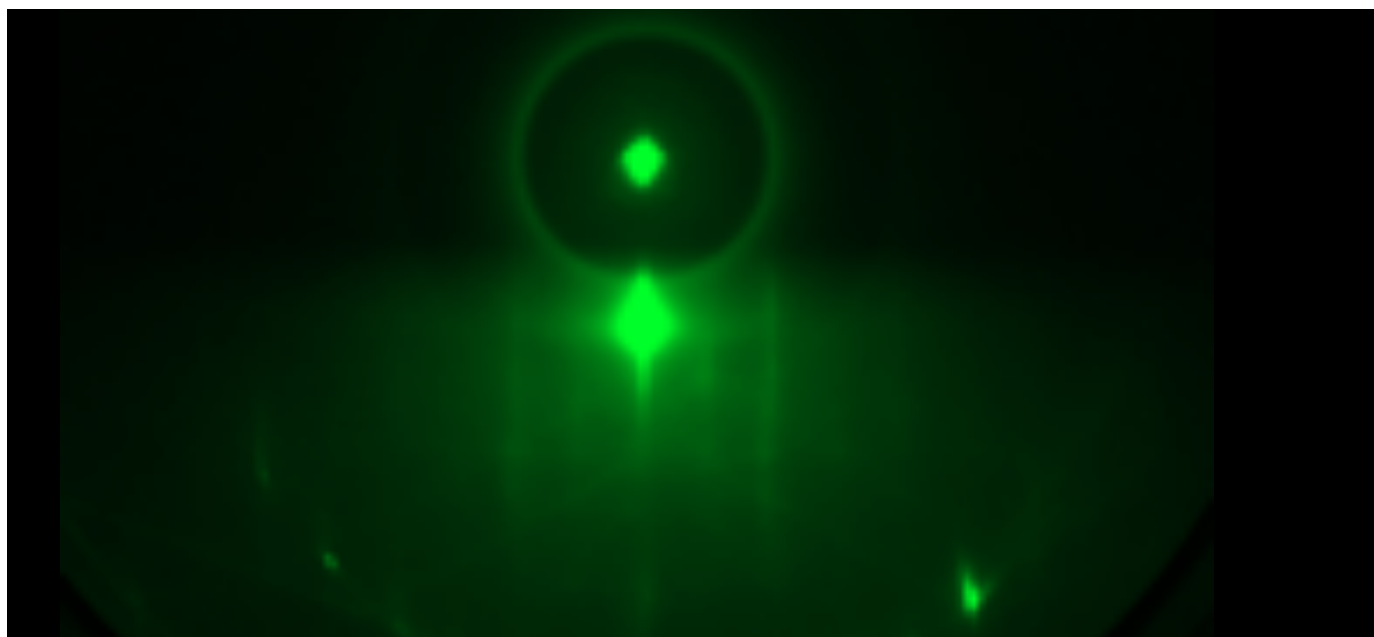
Data from seismic sensor networks are automatically processed to detect a variety of sources such as underground explosions, volcanic eruptions, induced microfractures, road usage, footsteps, etc. The quality of automatic detection depends on a large number of data processing parameters that interact in complex ways. The largely manual process of determining optimal parameters is painstaking and doesn't guarantee optimal configuration settings. Yet, achieving superior automatic detection of seismic events is closely related to these parameters.

We automated parameter tuning by developing automated sensor tuning (AST) software that learns near-optimal parameter settings for individual parameters. Parameters for each sensor are dynamically changed to achieve an optimal balance between missing signals from events of interest and detecting false signals. The key metric guiding the dynamic tuning is consistency of each sensor with its nearest neighbors: parameters are automatically adjusted on a per-station basis to be more or less sensitive to produce consistent agreement of detections in its neighborhood. The overall goal is to reduce the number of missed legitimate events and the number of false event detections. Reducing false alarms early in the seismic processing pipeline will have a significant impact on this goal. Applicable both for existing sensor performance boosting and new sensor deployment, the completed project will provide an important new method to automatically tune complex remote sensing systems. Systems tuned in this way will achieve better performance than is currently possible by manual tuning, and with much less time and effort devoted to the tuning process.

This project addresses the difficult problem of seismic sensor deployment. The innovative solution to sensor self-tuning will extend current state of the art in both seismology and machine learning. The project will have a fundamental impact on remote sensing and event detection with a wide-reaching impact for many national security remote sensing applications, including seismic, space, and imaging.



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## Materials Science

R&D sponsored by the Materials Science Investment Area strives to discover new phenomena, to create new classes of materials with novel synthesis techniques and processing approaches, and to understand and control materials' structures and properties. The goal is to foster a bold, vibrant, ground breaking, materials science base of world-renown, which serves as the foundation for developing the critical and differentiating technical capabilities that will be needed in the future to support our national security missions.

*The image above depicts a reflection high-energy electron diffraction pattern of the surface of a beta gallium oxide single crystal. The streaks and spots along a ring are indicative of a smooth and well-ordered surface that is appropriate for epitaxial growth. Development of these novel power semiconductor materials will serve as a platform for next-generation power electronics for energy security. (Project 191190, Fundamental Science of Doping and Defects in Ga<sub>2</sub>O<sub>3</sub> for Next Generation Power Semiconductors)*

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## Additive Manufacturing: Predicting the Performance and Reliability of Laser Engineered Materials

180901 | Year 2 of 3 | Principal Investigator: J. D. Sugar

### Project Purpose:

Opportunities for rapid qualification and engineering materials reliability exist in additive manufacturing (AM) because fully functional parts are built in a single operation one layer at a time. It is, therefore, possible to dynamically change and correct the manufacturing recipe to meet requirements. In comparison, conventional manufacturing processes are subtractive with several steps at different geographic locations. When one step is done incorrectly, an entire part must be scrapped since material cannot be fixed or added back. AM is inherently a nonequilibrium process with complicated simultaneous thermal and mass transfer. The question is how do rapid solidification, thermal gradients, and compositional gradients interact to cause the observed microstructural variation in AM parts? Our hypothesis is that the thermal history measured at each point in a part during manufacturing and the resultant microstructural variations are highly correlated, and knowledge of one is predictive of the other. We will use: 1) diagnostic sensors that measure the thermal history of a part during manufacturing, 2) analytic microscopy and mechanical testing to characterize microstructure and properties, and 3) finite element to mesoscale modeling to predict the evolution of properties, residual stress, and microstructure during AM processing. This study provides the first steps towards a fundamental understanding of the immediate and long-term performance of AM parts, which is required for their use in high consequence environments. A successful microstructural and property predictive capability for AM will potentially lead to materials qualification at the time of manufacturing “on the fly” without additional testing steps (i.e., “born certified”).

AM is receiving great interest within the NNSA complex for the possible production of weapons components. However, not much has been done to verify and qualify AM materials for those components. This project will contribute to the fundamental understanding of AM processes needed to assess whether these materials may be suitable for weapons reserve-quality parts.

## Compliant Nanoepitaxy: The Next Materials Revolution

180899 | Year 2 of 3 | Principal Investigator: S. R. Lee

### Project Purpose:

Sandia's pioneering contributions to lattice-mismatched semiconductor materials have seeded a ~40-year-long technology revolution in strained-layer heteroepitaxial devices—devices that now underpin optoelectronics based telecommunication technology, strained-silicon based microprocessors, and light emitting diode based solid-state lighting (SSL). While these achievements might suggest that the zenith of strained-layer materials R&D has passed, the cover article of the February 2014 Materials Research Society Bulletin asserts exactly the opposite: the confluence of elastic-strain engineering and nanotechnology places us instead at the beginning of a new era where nanostructured manipulation of strain in three dimensions will yield revolutionary new materials solutions. However, emerging research in this area often focuses on rapid application to devices, and not the fundamental materials science understanding needed to fulfill this concept. We will fill this knowledge gap via in-depth experimental and theoretical studies of compliant nanoepitaxy, focusing on nanostructure shape, composition, strain, and defect content. The model system proposed for study comprises  $\text{In}_{[x]}\text{Ga}_{[1-x]}\text{N}$  alloys grown on nanopatterned GaN. While these alloys promise efficient light emission and absorption spanning all visible wavelengths, high-energy-efficiency materials operating at green wavelengths and longer remain outside the reach of planar epitaxy because of extreme lattice-mismatch strains on GaN substrates ( $|d|/l=2.1\text{--}9.8\%$  for  $x=0.2\text{--}1.0$ ). Compliancy-based control of strain enabled by nanoepitaxy could unleash the full energy efficiency promise of these alloys by raising indium compositions in the alloys while simultaneously eliminating materials defects. This project seeks to leverage Sandia's unique combination of scientific expertise and state-of-the-art facilities to accelerate discovery in the emergent field of compliant nanoepitaxy and advance our knowledge of nano-enabled strain engineering, thereby creating innovative materials for applications in power electronics, photovoltaics, SSL, and beyond.



## Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials

191194 | Year 1 of 3 | Principal Investigator: H. Fan

### Project Purpose:

Energetic materials (EMs) exhibit inconsistencies in their performance/behavior due to the variety of production methods used to produce EM powders and the variability inherent within each processing method. The inability to reliably control morphology (size, shape) of EM particles on a production scale has made it challenging to reproduce specific chemical and/or physical characteristics, and increases expense and risk for applications using these materials. Thus, there is a pressing need to more reliably formulate EMs with greater control over morphological properties. We propose to use the cooperative self-assembly method, pioneered at Sandia to control the nucleation and growth of inorganic nanocrystal, to tailor structure and morphology of EMs. We will extend this method to generate EM particles with well-defined size and external morphologies using EMs that are both prevalent in the stockpile and present interesting reprocessing challenges. Through controlled EM self-assembly, we intend to understand fundamental science on how molecular packing influences EM structure and morphology. The self-assembled processes developed to engineer EM could potentially eliminate future lot-to-lot discrepancies by providing a trusted and reproducible method for reprocessing EMs. In addition, these studies will enable improved margin quantification for energetic components and could enable prediction of EM reliability.

This project will use Sandia-developed self-assembly techniques to develop new fundamental understanding of unexplored areas concerning how molecular self-assembly influences morphology in EM particles and how this control corresponds to performance of the materials. A successful project would enable new directions in EM reformulation and could lead to a trusted, reproducible EM production method to address nuclear weapon mission needs.

## Electrochemical Model of Humidity-Driven Corrosion

191187 | Year 1 of 3 | Principal Investigator: E. J. Schindelholz

### Project Purpose:

Atmospheric corrosion critically impacts the performance of engineered materials, components, and systems across Sandia's mission space. Current lifetime prediction strategies, such as accelerated tests and empirical models, can provide a qualitative picture of corrosion performance but oftentimes fall short of quantitative prediction. Achieving the latter would improve the operational assurance of high consequence, extended-life systems susceptible to atmospheric corrosion, such as the aging stockpile and used nuclear fuel storage containers. Advancement is hindered by lack of mechanistic understanding of the interrelationship between environment, the state of an exposed metallic surface, and its electrochemical response. A critical question in this regard is: what are the physicochemical characteristics of electrolyte features that develop on atmospherically exposed surfaces essential for the initiation and propagation of corrosion?

Here we seek to address this question for the case where hygroscopic surface contaminants, such as atmospheric particles and manufacturing residues, drive corrosion by humidity sorption to form electrolyte microdroplets (humidity-driven corrosion). This case is typical for climate-controlled or sheltered environments representative of stockpile and other national security system conditions. Current models developed for corrosion under larger electrolyte features that form in outdoor conditions (e.g., raindrops) do not capture the phenomenology reported under this microdroplet regime. This project aims to understand the role of sorbed water layers inherently present on surfaces and external to drops and their characteristics relevant to this observed behavioral divergence. A combined multiphysics modeling and experimental approach will be taken. The results will allow more accurate interpretation and quantitative prediction of humidity-driven corrosion.

This work will extend the current electrochemical model of atmospheric corrosion under macroscopic drops to the microdroplet regime. For the first time, the role of the electrolyte layer external to the drops will be considered and defined. The model and toolset developed will create a differentiating capability for electrochemical study of atmospheric corrosion.



## Engineered Reliability via Intrinsic Thermomechanical Stability of Nanocrystalline Alloys

180900 | Year 2 of 3 | Principal Investigator: N. Argibay

### Project Purpose:

Nanocrystalline metals have demonstrated clear advantages in strength, wear resistance, and fatigue tolerance over commercially available structural alloys. However, existing nanostructured alloys remain impractical for mission critical applications primarily due to their propensity to undergo rapid microstructural evolution upon application of thermal or mechanical load (even at room temperature). This microstructural evolution renders them unreliable and precludes fabrication in bulk forms. We have identified a novel approach to alloy design that renders certain binary alloys intrinsically stable, resulting in a new class of alloys inherently impervious to abnormal thermal environments, large cyclic thermal stresses, and loss of wear-resistance in electrical-tribological components. Recently, several groups have proposed models for stabilization of binary nanocrystalline alloys, and they have independently confirmed profound thermal stability: nanocrystalline grain size is maintained after weeks at 1100 °C (Massachusetts Institute of Technology, W-Ti), or after hours at 97% of melting (Army Research Lab, Cu-Ta). In the MIT model, grain boundary stabilization via segregation of immiscible solute creates a localized thermodynamic equilibrium that eliminates the driving force for grain growth. While there are important energetic distinctions between the different models for stabilization, they all disregard the destabilizing role of mechanical loading. The remaining scientific mystery to be unraveled is the interplay between mechanical stress/strain and grain boundary motion in the context of a segregation-stabilized nanocrystalline alloy. We propose to establish this link, initially focusing on alloys for electrical contacts (applicable to many components of interest). Such permanently stable alloys would be broadly transformative for applications such as transportation lightweighting and electrical contact technology for wind power.

## Engineering Bioelectronic Signal Transduction using the Bacterial Type III Secretion Apparatus

173670 | Year 3 of 3 | Principal Investigator: D. Y. Sasaki

### Project Purpose:

Engineering efficient methods for living systems to transfer electrical energy to nonliving systems, at relevant size scales, continues to challenge our knowledge of materials and biology. Our goal, in collaboration with the University of California-Berkeley, is to enable signal transduction between cells and inorganic materials, using controlled electron transport as the energy transfer mechanism. We envision using the cell as a living battery, providing a set of environmental signals to trigger synthetic biological networks that divert intracellular electron transport pathways to inorganic extracellular structures. Conversely, changing electron influxes could guide cellular responses. It is challenging, however, to precisely engineer nanostructured materials to achieve controllable catalytic or electronic properties and connect them with biological energy sources. Our approach to this problem is to engineer protein scaffolds, taking advantage of the native recognition, selectivity and self-assembly properties of these nanoscale building blocks as well as their native intracellular localization patterns. We are using a type III secretion system (T3SS) needle protein from *Salmonella enterica*, PrgI, as a template for metal nanowire synthesis for biosensing and bioenergy applications. Our strategy is transformative as there are few examples of devices that interface live cells with micro/nanocircuitry to extend the native functionality of biological systems.

This research provides a novel approach to electronically couple cellular systems with man-made devices, and creates a pathway toward bio-based electronic power supplies that could benefit battlefield equipment, surveillance systems, and health monitoring for DoD and DHS, and alternative energy sources for DOE.



## Fluxional Monomers for Enhanced Thermoset Materials

193378 | Year 1 of 2 | Principal Investigator: B. H. Jones

### Project Purpose:

We propose to design and create novel monomers that incorporate fluxional chemistry to alleviate the residual stresses that plague thermoset materials. Thermoset materials have been used for over a century as adhesives, encapsulants, and structural materials in a variety of applications, including many nuclear weapon components. Their performance, however, is limited by internal stresses imparted during processing that can cause failure during operation and aging. The conversion of a thermoset monomer to its final polymeric state is accompanied by drastic physical changes in the material, including gelation, vitrification, and volumetric contraction, which intersect with processing constraints such that the final product exists in a nonequilibrium state characterized by residual stress. Residual stresses are typically minimized through optimization of cure schedules or addition of inert fillers, yet there are practical limitations and drawbacks to these strategies. We will employ a novel chemistry-based solution to address this problem. Certain chemical functionalities involving cyclopentadiene-metal bonds exhibit extraordinarily low energy barriers to rearrangement among a diverse set of bonding modes. The incorporation of such functionalities into the network structure of thermosets offers the potential to exploit these spontaneous rearrangements as a mechanism for stress relaxation. In 2016, we synthesized a model thermoset based on a traditional epoxy resin reacted with a fluxional curing agent. This model material was found to exhibit reduced cure stress, as well as substantially enhanced stress relaxation behavior at elevated temperature. We intend to expand this concept to include a suite of traditional thermoset materials. In addition, we will explore several hypothetical mechanisms by which fluxional motion and its associated benefits to stress relaxation may be activated in glassy thermosets to reduce thermal stresses. Due to the generality of this chemistry-based approach, we anticipate that our success will have far-reaching impact across the many thermoset systems used within and beyond Sandia.

## Fundamental Science of Doping and Defects in $\text{Ga}_2\text{O}_3$ for Next Generation Power Semiconductors

191190 | Year 1 of 1 | Principal Investigator: J. Ihlefeld

### Project Purpose:

The purpose of this project was to investigate the fundamental science of growth of gallium oxide ( $\beta\text{-Ga}_2\text{O}_3$ ) with respect to next generation power semiconductor applications. If successful, the necessary growth conditions for  $\beta\text{-Ga}_2\text{O}_3$  would be developed enabling investment in more fundamental research in doping of materials, ultimately leading toward power device research. Power electronics are vital components of energy storage and control systems. Large silicon-based electronics have been used in switching and conditioning applications, but require cooling, operate at low frequencies, and therefore, limit efficiency. Silicon carbide (SiC)- and gallium nitride (GaN)-based power electronics have matured into commercial devices and possess advantages over silicon in operation temperature owing to wider bandgaps and operate at higher frequencies GaN owing to high carrier mobilities. This notwithstanding, future applications and DOE goals seek devices with higher breakdown strengths and operation temperatures in excess of 200 °C. This necessitates the development of a new power semiconductor material.

$\beta\text{-Ga}_2\text{O}_3$  possesses promising intrinsic material properties to meet this goal. Combining a wide bandgap (~4.8 eV), high electron mobility, and large electrical breakdown (8 MV/cm) strength,  $\beta\text{-Ga}_2\text{O}_3$  possesses a figure of merit 4X and 7X that of GaN and SiC, respectively. To be viable, however, fundamental knowledge of the doping, defect chemistry, and dopant activation mechanisms must be established. To date, this knowledge is lacking owing to incorrect assumptions valid in semiconductors being translated to oxides. In response, we developed a capability to grow epitaxial  $\beta\text{-Ga}_2\text{O}_3$  films by reactive oxide molecular beam epitaxy, which is necessary for future device exploration.

Gallium oxide holds great promise as a future power semiconductor, but understanding of fundamental material properties is in its infancy. This project utilized Sandia's unique oxide and semiconductor strengths to develop the capability to grow this material that is necessary to realize it for future mission needs in energy and power management.





## Harnessing Multiscale Periodicity of 2D-Crystals for Flexible Adaptable Broadband Optics

173124 | Year 3 of 3 | Principal Investigator: T. E. Beechem, III

### Project Purpose:

The library of isolated 2D crystals grows daily. Beyond graphene, atomically thin nitrides, oxides, and transition metal dichalcogenides (e.g.,  $\text{MoS}_2$ ) along with many others are now available and routinely stacked to create hybrid 2D solids. Importantly, when 2D crystals are combined, properties change. The mobility of graphene, for instance, is greatly improved when overlaid on hexagonal boron nitride. Similarly, arbitrarily stacked graphene transforms from a broadband to bandpass optical absorber. Such changes occur because of interactions between atomic layers. Leveraging the promise of 2D materials, therefore, necessitates the ability to understand the properties of not only the layers themselves but also their interactions with the environment. In response, this effort has investigated interlayer interactions in 2D solids identifying their impact in everything from material synthesis to power handling capability. This project identified many ways that these interlayer interactions impact 2D materials properties and resulted in several new tool set and synthesis capabilities for the study of 2D materials.

## High Fidelity Modeling of Ionic Conduction in Solids

173121 | Year 3 of 3 | Principal Investigator: F. P. Doty

### Project Purpose:

Thallium bromide has the properties to become the leading radiation detection semiconductor. It has not yet been deployed due to a short lifetime of only hours to weeks. While the rapid structural deteriorations must come from ionic conduction under operating electrical fields, detailed aging mechanisms have not been understood. As a result, progress to extend lifetime has been limited despite extensive studies in the past. We have developed new atomistic simulation capabilities to enable study of ionic conduction under electrical fields.

Our combined simulations and experiments indicate that dislocations in TlBr climb under electrical fields. This climb is the root cause for structural deterioration. Hence, we discovered new strengthening methods to reduce aging. Our new atomistic simulation approach can have broader benefit to other DOE/NNSA programs including battery research.

## High Power Solid-State Li-ion Batteries through Interface Engineering

191191 | Year 1 of 3 | Principal Investigator: F. El Gabaly Marquez

### Project Purpose:

The purpose of this project is to understand the origin of the high resistance that solid-state Li-ion batteries have at the interfaces between the components which hinders their power capability. This project seeks to identify and isolate the problem, then focus on resolving or minimizing the interfacial resistance and achieving enhanced power delivery (high current). This will enable the fabrication of relatively high power solid-state batteries that can be integrated with other electronics of interest to Sandia's national security missions, such as sensors, power harvesting, information processing, and antennas. Solid-state batteries are attractive because of their extremely long shelf and cycle life, small footprint, and resilience to extreme environmental and radiation conditions.



## Improved Mechanical Performance and Reliability of Radical-Cured Thermosets

180902 | Year 2 of 2 | Principal Investigator: E. M. Redline

### Project Purpose:

We set out to investigate to what extent mechanical and fracture properties of chain-polymerized thermosets can be improved by increasing network homogeneity using a novel approach based on controlled radical polymerization (CRP). Previous efforts in improving mechanical performance of thermosets focused on using additives such as particles, but recent research suggests that this particular class of thermosets is less receptive to additive toughening because of poorly developed cross-link network structure. Thus, an approach that focuses on network structure can potentially improve mechanical and fracture properties of the neat materials as well as those toughened using traditional additive strategies. The success of this project will ultimately allow UV-curable thermosets to be used in place of thermally cured/post-cured epoxies, thereby eliminating problems from thermal expansion mismatch.

While previous research has shown the potential of CRP to improve mechanical performance, the connections between the monomer chemistry, polymerization conditions, network structure, and mechanical properties remain largely unexplored. In order to enable applications of these materials, a quantitative understanding of polymerization reaction kinetics, extent of cure, network heterogeneity, and mechanical performance is essential. We have carried out such investigations using both experiments and simulations for two distinct monomer chemistries. We initially planned to also investigate the effects of additives in these materials, but experimental results showed an unexpected and interesting dependence of mechanical properties on both monomer chemistry and cure temperature history. We, therefore, shifted focus slightly to investigate these effects in detail during the latter part of the project.

In addition to demonstrating the feasibility of using controlled radical polymerization as a method for improving mechanical performance, a key goal of this project was to establish the workflows and techniques needed to study such systems via both experiment and simulation. This lays the groundwork for future investigations of these materials for a variety of national security applications, as well as studies of foams and polymer degradation.

## In Situ Study of Surface-Mediated Explosive Degradation using Surface Enhanced IR-Vis Sum Frequency Generation

173118 | Year 3 of 3 | Principal Investigator: D. Farrow

### Project Purpose:

Degradation of explosives at the bridgewire/explosive interface, where the bridgewire initiates detonation by plasma induced shock, is known to affect component performance. It has been observed that losses of <1% of total material in a bridgewire detonator can change function time and substantially reduce component lifetime. Two proposed mechanisms are: 1) low levels of ionizing radiation generate free electrons in the bridgewire that cleave a N-O bond in the explosive at the bridgewire interface and 2) chemical reactions at the metal interface (e.g., corrosion), bringing reactive species in contact with the explosive. Furthermore, products of explosive degradation may also corrode the bridgewire. No tool currently exists for in situ identification of short-lived intermediates at a buried interface. Current methods are only sensitive to bulk material (Raman), cannot access the organic/metal interface (mass spectroscopy) or cannot detect species in low concentration (IR-Vis sum frequency generation [SFG] spectroscopy).

We will build a novel platform to directly observe low concentrations of reactive species at buried organic/metal interface for the first time. We will improve on the state of the art by: 1) employing heterodyne detection of the IR-Vis SFG (HSFG) signal from an explosive/ metal film interface and 2) use the metal/film interface as a model for the explosive/bridgewire interface, exposing it to reactive stimuli and then probing surface mediated reactions in situ. If successful, we will make the first direct observation of reactive intermediates driving ionization and corrosion-mediated aging at the explosive/bridgewire interface.

This project will create a novel capability for in situ characterization of organic material aging within a few monolayers of a metal interface to identify intermediate species with life times of a few picoseconds at room temperature.



## Interfacial Effects on the Microstructure and Morphology of Energetic Materials

191188 | Year 1 of 3 | Principal Investigator: E. C. Forrest

### Project Purpose:

The microstructure and morphology of energetic materials strongly influences detonation properties. For example, porosity at the mesoscale affects output energy and the critical thickness needed to sustain detonation. Recent studies have demonstrated the importance of substrate properties on resultant microstructure of vapor-deposited explosive materials. However, the fundamental mechanisms by which substrate conditions alter these characteristics are poorly understood, leading to variation in and limiting the control over detonation properties. The energetics community is investigating relationships between microstructure and performance. The question inspiring this work derives from those efforts: what is the science that governs microstructure evolution and can we control it? Insight on this question could enable control of microstructure and hence, energetic performance.

We hypothesize that the interfacial surface energy and microtopography between substrate and explosive play a prominent role in the resultant microstructure and morphology evolution of the vapor-deposited explosive. However, the inherent variability of interfaces presents challenges in their study and has, to date, obfuscated their importance in resultant properties of energetic materials.

We seek to engineer, and ultimately, leverage interfacial characteristics at atomic-to-microscopic length scales to isolate and study individual effects on the properties of explosive films created with physical vapor deposition. We are investigating the role of surface energy and topography on properties of vapor-deposited films of pentaerythritol tetranitrate (PETN) through careful control of substrate conditions. Lithography and etching enables creation of well-controlled topography, while deposition of metal thin films enables augmentation of surface energy. The role of surface contamination at interfaces is also considered. Interfacial conditions are quantified using advanced surface science techniques, enabling phenomenological-based correlation to microstructure and resultant detonation properties.

Previous research sought to engineer porosity into explosive films following deposition using microelectromechanical systems (MEMS)-based fabrication techniques. Our research is unique in that we seek to alter and control energetic film properties through engineering of interfacial conditions prior to the deposition process.

## Microsensor Arrays for Energy Efficiency, Emission Monitoring and Explosives Detection

180835 | Year 2 of 2 | Principal Investigator: F. H. Garzon

### Project Purpose:

The purpose of this project is to develop ceramic electrochemical multi-sensors, integrated on a single chip, which will sense gases such as carbon monoxide (CO), hydrocarbon (HC), sulfur oxides (SO<sub>x</sub>), and nitric oxide emissions (NO<sub>x</sub>). These gases are ubiquitous emissions that result from the combustion of hydrocarbon fuels and are regulated by the US Environmental Protection Agency (EPA) and other international regulatory organizations with more stringent standards being enforced in the 2017 EU and EPA Tier III regulations. Dynamic measurement of emissions is essential feedback for optimizing combustion efficiency while minimizing emissions. Cost effective control and monitoring of these species requires new sensing technologies as traditional spectroscopic and/or chromatographic methods are expensive, bulky, and are often unsuitable for continuous unattended operation. The aforementioned molecules are also decomposition products of most explosives and provide unique signatures for their identification. The solid state electrochemical devices generate a voltage or a current that is proportional to the concentration of the gas species. Unlike liquid electrolyte-based sensors, they exhibit excellent long term stability and solid electrolyte sensors can operate at elevated temperatures (400-800 °C), thus making them excellent candidates for in situ applications. The multi-sensor arrays detection principle is based on nonequilibrium, differential electrocatalysis, and will produce a voltage signal proportional to concentration. The devices will measure combustion process emission gases and the HC, NO<sub>x</sub>, and CO decomposition products of the pyrolysis of nanoparticles and molecules of explosives.

The microfabrication of the nontraditional materials requires significant process development and the development of the devices requires significant cross-disciplinary expertise in solid state electrochemistry and materials science. If successful, this technology has numerous potential applications that would benefit a number of energy and national security missions, such as clean energy generation, environmental monitoring, as well as chemical and explosive detection.



## Microstructural Modeling of Brittle Materials for Enhanced Performance and Reliability

195883 | Year 1 of 3 | Principal Investigator: M. C. Teague

### Project Purpose:

Understanding failure in brittle materials, which are ubiquitous in the nuclear weapons stockpile, is critical to predicting and ensuring performance and long-term reliability in service. Current practice is to employ engineering judgment with continuum-scale finite element (FE) modeling to design to a maximum stress below the critical failure stress. Unfortunately, the conservative safety factor employed to compensate for the unquantifiable uncertainty in legacy continuum-scale FE model stress predictions is becoming more and more impractical for increasingly complex designs and/or with materials pushed to their limits. To better quantify uncertainty and design margins, higher fidelity stress modeling is required. Recognizing that brittle materials fail well below their theoretical bond strength from microstructure-scale defects, the objective of this project is to develop and implement a microstructure-scale FE modeling capability to predict stress with higher fidelity on the microscale, including the capability to predict the stress intensification associated with continuum-scale stress field interactions with microscale defects.

This project will create an experimentally validated microstructure modeling capability to enable failure predictions for brittle materials. A unique combination of FE modeling, microstructure characterization, and microstructure-scale stress mapping will be used to create the microstructure modeling capability. If successful, this effort will contribute to the tools and understanding necessary to provide assurance that a brittle component in a high-consequence application is fully functional over its intended lifetime.

## Molecule@MOF: A New Class of Optoelectronic Materials

180898 | Year 2 of 3 | Principal Investigator: A. A. Talin

### Project Purpose:

The purpose of this project is to develop a new family of materials with highly tunable electronic properties based on the concept of guest molecule adsorption into the pores of a metal-organic framework (Guest@MOF). MOFs are an emerging family of metal-organic coordination compounds with regular molecular size pores that form an inherent part of the crystalline lattice. MOF-based electronics have potential national security applications in novel computing devices, reconfigurable electronics, sensors, and energy conversion. We have discovered that by introducing guest molecules into the pores that interact electronically with the framework we can dramatically change the electronic and optical properties of the resulting Guest@MOF material. Using our initial platform based on TCNQ (tetracyanoquinodimethane) infiltration into the porous framework  $\text{Cu}_3(\text{BTC})_2$  (BTC – benzene tricarboxylate), we have demonstrated that the emergent electronic conductivity is due to electron transfer from the MOF to the TCNQ guest. We have also shown that such materials may be useful for thermoelectric energy conversion due to their very low thermal conductivity. As we continue to explore the  $\text{TCNQ}@\text{Cu}_3(\text{BTC})_2$  and related systems, we have also initiated an intense effort to modulate the electronic conductivity and optical properties of inherently conducting MOFs such as  $\text{Ni}_3(\text{HITP})_2$  (HITP – hexaiminotriphenylene). Our preliminary tests suggest this system can exhibit majority n-type carriers, and by using the Guest@MOF approach, we hope to achieve sufficiently high conductivity to make the material promising for polymer-based thermoelectric energy conversion. All of our experimental work is carried out in close collaboration with modeling efforts that both guide the experiments and help explain observations. The coupling of theory and experiment improves our understanding and facilitates discovery of these new Guest@MOF materials with technologically useful properties.



## Multi-Resolution Characterization and Prediction of Environmentally-Assisted Intergranular Fracture

173116 | Year 3 of 3 | Principal Investigator: R. A. Karnesky

### Project Purpose:

Material fracture in the US costs over \$119 billion annually. Environmental influences such as hydrogen, irradiation, and high temperatures render ductile alloys susceptible to brittle fracture. For Sandia's NNSA and other national security sponsors, unexpected component failures lead to unacceptable consequences such as the release of flammable or radioactive chemicals. These failures impact gas transfer systems, hydrogen for transportation, and nuclear power generation and waste storage.

At present, however, most procedures for managing materials in harsh environments rely on extensive experimental databases in the form of empirical crack growth equations, and are implemented into structural analysis codes. These procedures cannot be reliable without thorough experimental data because of complex interactions of environmental influences with deformation mechanisms and microstructure. We propose a validated computational capability to move beyond the empiricism of current methods.

Our multiphysics, multiresolution framework couples simulations and unique experimental techniques at multiple length scales. Applying this coupling to a thoroughly understood material, the resulting model can predict transient fracture resistance. Deliverables open new core capabilities needed by DOE and NNSA for interpreting effects of environmental variables and their interactions with microstructure.

Novel atomistic and continuum models predicted grain boundary (GB) structures and energies, the segregation of hydrogen to GBs, and the work to separate GBs. Atom-probe tomography was used to measure segregation experimentally. In situ and 3D transmission electron microscopy were used to measure dislocation structure and activity near the boundaries. Environmental testing determined how different distributions of segregants and GB structure changed fracture properties.

## Novel Cathode Materials for Large-Scale Electrical Energy Storage

177964 | Year 3 of 3 | Principal Investigator: D. F. Sava Gallis

### Project Purpose:

Environmental concerns and the limited resources of fossil fuels, in conjunction with energy security needs, have increased the importance of renewable technologies (wind and solar) in the electrical energy landscape. Since renewable energy sources are intermittent, integration with the grid requires robust energy storage solutions to tailor power generation and supply to demand. Electrical energy storage is well equipped to balance the dynamics of demand and supply, however, very few technologies can meet the cost-performance targets required for widespread implementation. Existing electrochemical technologies for large-scale storage suffer several limitations: modest cycle life and efficiency (lead acid batteries), low charging rates and efficiency (Na-S, Na-metal halide), and prohibitive costs (Li-ion batteries).

The purpose of this project is to develop novel materials for large-scale electrical energy storage. In order to attain both fast cycling and enhanced storage capabilities, we are focused on implementing metal-organic frameworks (MOFs), a class of materials virtually unexplored in the large-scale energy storage arena. MOFs are inherently highly porous and, therefore, fast ion insertion and removal during cycling can be achieved. Additionally, multi-electron transfer is possible due to the hybrid inorganic-organic nature of these materials. Since both the metal and organic ligand can be redox-active, this can lead to higher energy storage per gram of material. Emphasis is placed on establishing: 1) a methodology to successfully fabricate MOFs-based coin cell batteries capable of running over hundreds of cycles and 2) the structure-function relationship in these systems through the fundamental understanding of the mechanism for ion insertion/extraction, correlated with the electrochemical performance. This project is designed to be successful via a multidisciplinary approach of materials synthesis and characterization and battery design and testing expertise.





## Phonon Scattering at Mobile Ferroelastic Domain Walls: Toward Voltage Tunable Thermal Conductivity

173117 | Year 3 of 3 | Principal Investigator: J. Ihlefeld

### Project Purpose:

The challenge addressed in this project was to actively modify thermal conductivity in a solid-state material over a broad temperature range using nonmechanical stimuli, which has been an elusive technological goal. This will enable active and low-power thermal emission and heat energy control. To date, altering thermal conductivity in a material at noncryogenic temperatures had only been achieved by applying a mechanical strain, by traversing a narrow phase transition, or by changing the chemical composition of the material itself. The solution proposed in this project was to achieve voltage tuning of thermal conductivity by harnessing mobile coherent interfaces (domain walls) in ferroelectric materials to scatter heat carrying phonons. By adjusting domain wall spacing to be smaller than the phonon mean free path through preparing thin films, phonon-domain wall scattering becomes the dominant mechanism leading to manipulation of thermal conductivity. Electric fields can alter the configuration and density of these interfaces and result in tuning of thermal conductivity. We studied  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  thin films where domain wall type and density can be deterministically controlled. We developed an approach to tuning thermal conductivity by gaining an understanding of the variables controlling phonon scattering at domain boundaries. Using empirical results and phase field modeling, we demonstrated field-tunable thermal conductivity at noncryogenic temperatures in both a bilayer ferroelectric thin film and a ferroelectric film of uniform composition. Further, we gained a new understanding of different phonon scattering mechanisms in these materials by studying alloy composition effects in order to maximize the effectiveness of the thermal tuning behavior.

Demonstration of altering thermal conductivity at room temperature in a nonmoving solid-state material had not previously been accomplished. To be exploited for applications this phenomenon needed to be demonstrated and understood, which was our primary accomplishment.

## Predicting the Multiscale, Mechanical Response of Additively Manufactured Materials across a Wide Spectrum of Loading Conditions

178667 | Year 3 of 3 | Principal Investigator: D. P. Adams

### Project Purpose:

Developing a fundamental understanding of a material's mechanical behavior has traditionally relied on time-consuming and costly experimental characterization. However, as microstructures and interfaces become more exotic due to novel fabrication techniques (e.g., additive manufacturing), assured performance will come to rely on strong coupling between experiments and modeling of material behaviors. Predictive modeling must now incorporate the detailed microstructural 'elements' present in a starting material. Furthermore, modeling should be able to predict mechanical properties for a wide range of loading conditions in order to assure that novel microstructures will have acceptable responses to mission-relevant environmental conditions.

Toward this end, this project: 1) examined whether homogenization and multiscale theory can predict the dynamic mechanical behaviors of additively manufactured materials and 2) elucidated how the produced complex microstructures affect mechanical response. Our research of these fundamental questions relied heavily on implementation of Sandia's state-of-the-art direct numerical simulation (DNS) technique to evaluate the grain-scale response of nonuniform microstructures, and coupling of those results to macroscale models. Building from Sandia's crystal-plasticity models and fed by experimental evaluations, grain-scale behavior was determined and then coupled to larger-scale models predicting structural response to a range of strain rates in the quasistatic regime. Validation experiments were completed to contrast different predictive modeling approaches. Our approach extended beyond simple uniaxial loading (in compression or tension) to include complex axial-torsional loading.

This project has improved Sandia's ability to predict mechanical response of materials having complex microstructures. This applies to different materials made by additive manufacturing processes and also to materials formed by other emerging processes. This puts us in a better position to assess and assure performance and qualify new, candidate materials for mission-relevant environmental conditions.



## Quantum Nanofabrication: Mechanisms and Fundamental Limits

191196 | Year 1 of 3 | Principal Investigator: G. T. Wang

### Project Purpose:

Semiconductor nanostructures exhibiting quantum-size effects represent the next frontier in nanophotonics and nanoelectronics, capable of enhanced performance and new functionalities. However, the controlled fabrication of nanostructures in the ~sub-10 nm quantum size regime has proved extremely difficult using current approaches, limiting the potential of quantum nanostructure enabled devices.

Quantum size effects themselves can potentially be exploited to precisely control nanofabrication. By influencing the energies of electronic states, these effects will influence the susceptibility of the developing nanostructure to excitation by photons or electrons, and thus, to material addition or subtraction processes mediated by excited electronic states. Recently, we demonstrated for the first time the ability to create epitaxial nanostructures using just such a process: quantum-size-controlled photoelectrochemical (QSC-PEC) etching. PEC etching depends on light absorption, light absorption depends on bandgap, and bandgap depends on nanostructure size. QSC-PEC etching can thus self-terminate at a wavelength-determined size/bandgap. Sandia's pioneering work has already enabled ~5X narrower InGaN quantum dot (QD) ensemble energy dispersion than typical of standard strain-driven QD growth.

We believe that this new paradigm of "quantum nanofabrication" using quantum-size effects can potentially be the solution to the challenges of accuracy and precision in quantum nanostructure fabrication. Here, we propose to answer the key question of what the underlying, fundamental mechanisms of QSC-PEC etching are that determine its ultimate accuracy and precision. This will enable us to understand the scope of its ultimate applicability in emerging quantum nanostructures and nanodevices across a wide range of materials systems.

This high-risk, discovery-based research will enable a new foundational capability in quantum nanofabrication across a wide range of materials systems, with relevance to national security mission needs. It requires Sandia's unique synergy of capabilities in III-nitride and III-V compound semiconductors, nanofabrication, and nanocharacterization, positioning Sandia's leadership in this nascent field.



## Room Temperature Solid-State Deposition of Ceramics

177962 | Year 3 of 3 | Principal Investigator: P. Sarobol

### Project Purpose:

The ability to integrate ceramics with other materials is limited by high processing temperatures ( $>800\text{ }^{\circ}\text{C}$ ). A process to fabricate ceramic films at room temperature (RT) in solid state, aerosol deposition (AD) has been demonstrated in literature. High velocity ceramic particles impact on substrates, deform, and form films under vacuum. AD eliminates high processing temperatures and enables materials integration, where ceramics are deposited on metals, plastics, and glass at RT. AD films are reported to have excellent properties, equivalent to or exceeding conventional pressed/sintered ceramics. Anticipated benefits include improved ceramic integration, miniaturized magnetic circulators in radar applications, conformal capacitors, thin batteries, glass-to-metal seals, and transparent electronics for national security applications.

The fundamental mechanisms for ceramic particle deformation/bonding in AD are not understood and are needed to advance this technology. This project leveraged Sandia's existing experimental equipment and simulations capabilities to establish mechanisms and processing/microstructure/properties relationships. In FY 2015, we showed defective  $3\text{ }\mu\text{m}$  particles fracture whereas nearly defect-free,  $0.3\text{ }\mu\text{m}$  particles plastically deformed before fracturing in compression. Plastic deformation is possible when strain energy density in submicron particle is high enough to initiate nucleation of mobile dislocations. Thus, feedstock preparation by ball milling would introduce mobile dislocations and effectively lower the impact energy (particle velocity) needed for deformation. In FY 2016, Sandia's AD capability was brought online, deposition experiments were performed, and particle-particle bonding mechanisms were determined to be from tamping effect. Finally, we demonstrated aerosol deposited ceramic, metallic, compound, and composite coatings— $\text{Al}_2\text{O}_3$ ,  $\text{TiO}_2$ ,  $\text{BaTiO}_3$ ,  $\text{HfC}$ ,  $\text{Cu}$ ,  $\text{Ni}$ , etc. We also demonstrated materials integration by aerosol deposition of  $\text{Cu-BaTiO}_3\text{-Cu}$  alternating layers, relevant for capacitor applications.

This project established knowledge of fundamental mechanisms underlying formation of ceramic films by this room temperature process. A combination of experimentation and simulation were used to determine the fundamental mechanisms underlying the formation of a dense, structurally robust solid and establish relationships among processing, microstructure and properties needed for technological maturation in the future.

## Scanning Ultrafast Electron Microscopy for Charge Carrier Lifetime Imaging with High Spatial Resolution

173119 | Year 3 of 3 | Principal Investigator: J. R. Michael

### Project Purpose:

The purpose of this project was to develop, build, and use an innovative new scanning ultrafast electron microscope (SUEM) dedicated to probe active regions of semiconductor devices to determine the carrier lifetimes and infer the doping concentrations.

The prototype SUEM instrument includes a photocathode source that is excited by a laser; the sample is also excited by the same laser but with a variable time delay between the time that the beam electrons interact with the sample and the time that the sample is illuminated with a short pulse of laser light. This has been accomplished without degrading the performance of the scanning electron microscope. The construction of the SUEM has allowed the shortcomings of previously built SUEM instruments to be understood and possibly improved upon. Two important improvements are the use of microchannel plates for secondary electron collection and electron beam induced current (EBIC) mode in the pump probe configuration. The use of the microchannel plates allows the precise timing of the pump and the probe pulses to be determined. The use of EBIC signal collection modes is truly novel and has not been used with the SUEM in previous work. The use of EBIC allows a quantitative measure of the actual carrier currents within the sample to be determined and visualized. New and not entirely understood image contrast has been observed in the EBIC mode of operation.

Previously, scanning ultrafast electron microscope developments were directed mostly at understanding chemical processes. As a result of this work, the SUEM can be applied to semiconductor materials of importance to the NNSA and to the general semiconductor materials communities. The ability to image doped regions in semiconductor devices and to begin to determine the carrier lifetimes will enhance the way semiconductor materials are studied and will help our understanding of charge carrier dynamics.



## Sequential Design of Experiments for Accelerated Life Testing

195881 | Year 1 of 3 | Principal Investigator: C. King

### Project Purpose:

Accelerated testing has become a popular technique for extracting information about product performance within a reasonable and cost-effective time frame. As such, a significant proportion of the literature on accelerated testing in the field of statistics has focused on researching methods for designing accelerated test plans that yield the most precise estimates of target quantities (mean response, 99th percentile, etc.) given the available resources. Such test plans are called “optimal designs” and are usually heavily dependent on assumptions regarding the distribution of the response and the model relating the acceleration factor (temperature, voltage, etc.) to the response. In addition, the methodology used to develop these optimal designs usually assumes a large number of samples are present so as to utilize well-known mathematical results. The purpose of this project is to create a testing procedure that can be used when there is a lack of information regarding the response distribution and/or the acceleration factor model. The primary objectives are: 1) to investigate how the model form and response distribution inform optimal test designs as a function of the exact sample size rather than an assumed large sample and 2) to use the results of this investigation to inform the construction of a sequential testing procedure for use in settings where knowledge regarding the response distribution and the acceleration factor model is unavailable. The investigation will primarily be driven by simulation studies due to the complexity of the mathematics involved.

## Understanding Transport and Aging Mechanisms to Optimize Sandia’s Ion-Conducting Electrolytes for Energy Applications

191186 | Year 1 of 3 | Principal Investigator: A. Frischknecht

### Project Purpose:

To secure a sustainable, clean energy future, the US needs more efficient stationary energy storage and cleaner transportation energy sources. Cheap and efficient ion conducting separators are needed to improve efficiency and lifetime in fuel cells, batteries, and electrolyzers. Current state-of-the-art polymeric separators are made from Nafion, which is too expensive to be competitive with other technologies. Sandia has developed unique polymer separators that have lower cost and equivalent or superior ion transport compared to Nafion. However, there have been no long term reliability or performance studies of these separators. Further, rational design of new separators requires molecular-level knowledge, currently unknown, of how polymer morphology affects transport. We are using Sandia’s separators as a platform to investigate proton transport in polymers, and to focus on the potential of these separators to become the fuel cell membrane of choice. The science questions we will answer are: 1) why do Sandia’s current generation separators have such excellent transport properties, 2) what modifications can improve this performance, and 3) how does aging impact the transport and mechanical reliability of these separators? We are using a coupled approach including advanced polymer synthesis, experimental characterization from the molecular to continuum scales, polymer theory and simulations, and device testing to develop a scientific understanding of ion transport and aging in polymer separators. This research is different from previous research in both new methods and in the tightly integrated approach, as well as the new polymer chemistry. For example, we are developing a new method to use information from simulations to interpret experimental nuclear magnetic resonance data on the morphology of the separators. Additionally, we are systematically synthesizing a series of polymers and using many techniques to characterize them. The understanding we gain will allow us to modify the polymer architecture for optimum performance.



## Understanding and Overcoming Materials Challenges for AlN: A Scientific Foundation for Next-Generation Power Electronics

173122 | Year 3 of 3 | Principal Investigator: A. Armstrong

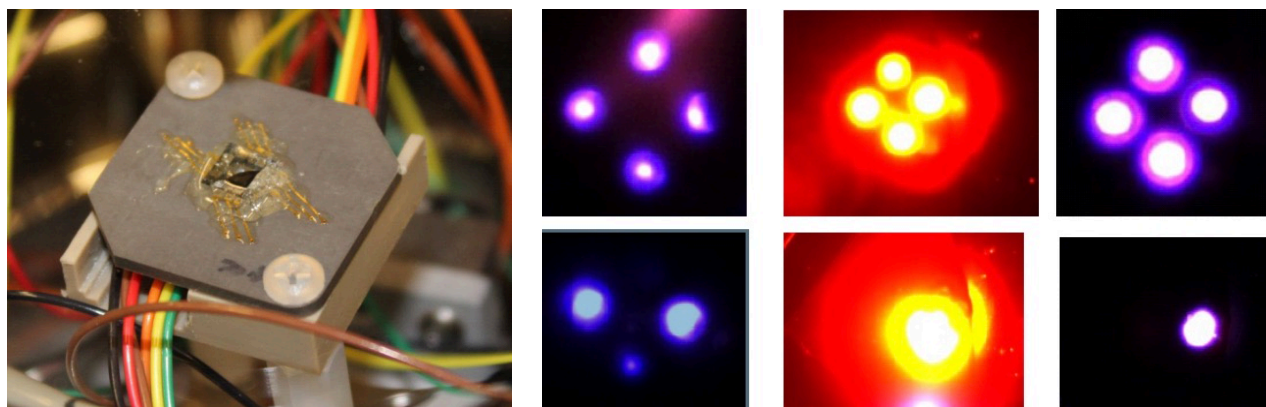
### Project Purpose:

The proposed research will lay the foundation for ultra-wide bandgap (UWBG) semiconductor material science by transmuting aluminum nitride with bandgap energy ( $E_g$ ) of 6.2 eV from an electrical insulator to an electrically conductive material with fully tunable conductivity type. This will enable a revolution in power electronics because the breakdown voltage ( $V_{br}$ ) grows rapidly with  $E_g$ . UWBG-based power switches with  $V_{br}$  upwards of 100 kV become plausible for enabling energy technology revolutions such as DC electrical grids with greatly improved efficiency. Aluminum nitride is attractive due to its large  $E_g$  and compatibility with existing semiconductor technology. However, AlN is electrically insulating and must be made conductive to function as an electronic material. Typical methods of controlling electrical conductivity for semiconductors (e.g., impurity doping and minimizing crystal defects) fail for AlN because thermodynamics drives spontaneous defect formation that completely compensates dopants. New methods must be discovered to control the electrical conductivity of AlN.

This project sought to demonstrate controllable electrical conductivity for AlN for the first time using the strong piezoelectricity and noncentrosymmetric lattice to produce electrical conductivity without dopants. Advanced defect spectroscopy was employed to understand the physical origin and properties of defects in AlN and mitigate their impact on electrical properties. Quantum kinetic theory was developed to assess electrical transport phenomena in AlN by treating the largely unexplored physics of carrier scattering in AlN including strong electron-phonon coupling and quantum memory effects.

Making AlN a functional electronic material requires surmounting new challenges attendant with large band gap that makes otherwise simple tasks difficult (e.g., doping). This project demonstrated electronic functionalization of ultra-wide band gap AlGaIn in highly scalable two-dimensional and three-dimensional geometries for the first time. By improving and controlling electrical conductivity in high Al content AlGaIn, we successfully harnessed its extremely large critical electric field to enable generation-after-next high voltage power electronics and high power radar device development.





## Nanodevices and Microsystems

The Nanodevices and Microsystems Research Foundation supports Sandia's mission by performing creative, leading edge, and high-impact R&D. This R&D strives to discover new phenomena at the nanoscale and microscale; and create or prove new concepts, devices, components, subsystems, and systems. Its objective is to foster a bold, vibrant, ground-breaking, science and technology base of world-renown as a means to developing the critical and differentiating technical capabilities that will be needed in the future to support our national security missions. The Nanodevices and Microsystems Investment Area seeks to: 1) increase our understanding of physical phenomena across the nanoscale to microscale, 2) develop innovative nanoscale and microscale devices, 3) achieve new methods of integration, and 4) realize novel microsystems-based complex systems.

*The above images illustrate: (left) a novel microplasma discharge device fabricated at Sandia's Microsystems and Engineering Sciences Applications Complex facility, developed for better understanding intense ultraviolet emissions. At right are microplasma images of 4-element arrays of a 100 micrometer diameter microplasma device. The images are with Ar, Ne, and He, from left to right. This research will aid eventual development of useful applications like photonics and chemical ionization/detection. (Project 173131, Fundamental Scaling of Microplasmas and Tunable UV Light Generation)*

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## A Compact, Spectrally-Tunable Source of Entangled Photon-Pairs for Quantum Sensing

192786 | Year 1 of 3 | Principal Investigator: I. Brener

### Project Purpose:

The use of entangled photons combined with spectroscopic, interferometric, and imaging techniques enables sensing beyond the limits of classical optics. Examples include chemical sensing with sub attomolar sensitivity, and spectroscopy with a low photon flux under noisy conditions. Entangled photon pairs are typically generated using nonlinear optical processes in nonlinear crystals, fibers, or waveguides. Unfortunately, because of photon statistics, these sources are nondeterministic in time and typically require wavelength multiplexing of different sources to achieve desirable high photon pair rates. Moreover, randomness of the photon wavelength in each pair means increased size and complexity of the overall system.

We propose a new source for generation of entangled photon pairs in the near infrared ( $\sim 1.5 \mu\text{m}$ ) based on semiconductor heterostructures (III-nitrides) coupled to metamaterials. This combination can create giant, gated, and tunable optical nonlinearities, thereby enabling control of the entangled photons wavelength and the ability to switch photon generation on/off using a bias voltage. The proposed source is a small, thin chip with easy, normal incidence input/output coupling (i.e., no waveguide alignment) that utilizes the core competencies in III-V semiconductor growth and processing at Sandia. Voltage control of the photon pair wavelength and the nonlinearity can be used to overcome some of the limitations of current generators (e.g., low photon rate and wavelength spread). If successful, we would create a new type of entangled photon pair source that would enable miniature quantum sensing systems and sensing/imaging at nonconventional, mid to near infrared wavelengths with entangled photons.

## A New Approach to Entangling Neutral Atoms

173130 | Year 3 of 3 | Principal Investigator: G. Biedermann

### Project Purpose:

We propose a new technique for entangling neutral atoms that will show feasibility of significant metrological gains. The principal motivation for harnessing entanglement in the context of quantum sensing is the superior scaling of sensitivity with atom number,  $N$ , when compared with classical sensing (e.g.,  $N$  versus  $\sqrt{N}$ , respectively). While the advantage with a small number of atoms is moderate, it reaches an order of magnitude improvement with only 10 atoms in that the same sensor precision can be reached in a time 10 times shorter. Neutral atoms are the most compelling candidate for quantum sensing with entangled systems because they have been broadly shown to make exceptional sensors. However, the fidelity of entangling two atomic qubits was previously limited to 75%, a number unsuitable for entangling many atoms.

The conventional approach to entangling neutral atoms uses resonant excitation to a Rydberg level, allowing atoms to interact via electric-dipole-dipole coupling. The primary limit to fidelity is thermal motion causing the exciting laser beams to imprint random phases on the quantum states and, thereby, degrade the coherence of the entangling interaction. By employing adiabatic evolution induced by a laser tuned off-resonance from a Rydberg level, the coherence can be much more robust. With our new approach, we predict two-qubit entanglement with fidelities near 99.8%. In addition, we will explore unique entangling operations beyond two qubits that are not easily accessible in other technologies. We anticipate multi-faceted impacts in both quantum sensing and computation.



## A New Paradigm in Chem/Bio Threat Detection: Evaluating Threats Based on Biological Function Rather than Chemical Form

191203 | Year 1 of 3 | Principal Investigator: W. F. Paxton

### Project Purpose:

Detecting chemical and biochemical species with high sensitivity and specificity is critical for identifying, attributing, and responding to chemical and biological threats. Conventional approaches to detect chem/bio agents rely on matching the chemical/spectroscopic properties of a sample to those of a known target, or selective binding to highly selective receptors (e.g., antibodies, aptamers, etc.). As such, these approaches are susceptible to false negatives by agents that have been deliberately modified to evade detection while retaining their toxicity or pathogenicity. For example, even single amino acid substitutions can significantly reduce and potentially eliminate the binding of a biotoxin to an antibody used for detection in a biosensor. Here, we propose a novel approach in chem/bio threat detection that identifies hazards based on their specific biological function, rather than on specific chemical signatures. Our approach is to integrate a set of functional membrane proteins and ion channels (often targets of chem/bio agents) into robust polymer bilayers on electronic sensory elements (silicon nanowire field effect transistors, [SiNW-FET]). Toxin-induced changes in biological function of specific membrane proteins due to threats—known and unknown—can be detected rapidly by the SiNW-FET device independent of identifying specifically what chem/bio agent is present. Moreover, this approach may be multiplexed on a single microchip for the detection of a range of threats based on the activity against different membrane proteins, each on an individual SiNW-FET element.

Our proposed approach has potential to revolutionize state-of-the-art biosensors. Insights from our research—even if unsuccessful—will have value to other efforts related to sensing, solid-liquid interfaces, and self-assembled materials.

## A Platform for Quantum Information and Large-Scale Entanglement with Rydberg Atoms in Programmable Optical Potentials

191211 | Year 1 of 3 | Principal Investigator: M. J. Martin

### Project Purpose:

Achieving large-scale entanglement and high-precision quantum gates in quantum systems could enable sensors with unprecedented precision, inform understanding of complex matter, and realize a quantum computer. Neutral atoms are well suited as building blocks of such a system, because their number can be scaled without undue difficulty, and interactions between the atoms (key to achieving entanglement) can be tuned via coupling to a high-energy atomic state and the spacing between atoms. To date, interacting neutral atom-based quantum systems with arbitrary center of mass control have utilized pairs of atoms. While few-atom ensembles are important for benchmarking entanglement, many-atom ensembles open the door to several important applications. Examples include: 1) clusters of entangled atoms for high-precision/resolution sensing, 2) a controllable quantum system to inform solutions to complex problems in condensed matter that are otherwise computationally intractable, and 3) large atomic arrays with controllable interactions to realize a quantum computer.

This project provides a flexible and controllable method for scaling the successes of two-atom experiments to many atoms. We investigate if arbitrary computer-controlled potentials can enable high filling-factor arrays of single atoms where the array configuration can be tailored to specific goals. We attack key limitations of scaling current experiments to many-atom arrays, specifically single-site loading and flexible control, via development of dynamically controllable holographic optical trap. Specific questions we will investigate in this project are the suitability of liquid crystal-based light modulators for creating dynamic traps, and if any limitations exist to scaling Rydberg atom interactions for entanglement beyond two atoms. Additionally, Sandia has the unique capability to control atomic interactions with an ultraviolet laser system. We will explore the creation of highly entangled states of more than eight atoms with rings and other geometries, where the programmable nature of the trap allows agile tailoring of the trapping geometry and thus the quantum properties of the system.



## Atom Traps on a Microfabricated Optical Waveguide Platform for Quantum-Limited Spin-Squeezed Magnetometry and Quantum Information Applications

180919 | Year 2 of 3 | Principal Investigator: Y. Jau

### Project Purpose:

The purpose of this project is to develop a new neutral-atom platform that utilizes optical evanescent fields from the light transmitted in a fabricated nano-waveguide to optically trap atoms in the well-defined locations. In this way, we can avoid complex free-space alignments for optical access of atoms, and this platform can be scalable and flexible. In addition, photons traversing the waveguide are confined to a region of space comparable to the absorption cross section of an atom, naturally making a very strong photon-atom interaction, which is of fundamental importance to photon-assisted quantum controls with atoms. Furthermore, this waveguide configuration, when combined with the ability to incorporate photonic-crystal optical elements, leads to exciting opportunities such as cavity quantum electrodynamics with record-setting atom-photon coupling and long-range atom-atom interactions mediated by photons. The ability to create complex structures on this "optical atom chip" would have important application to precision measurement (quantum sensing) and to quantum computing and communication technologies. To increase the likelihood of success with the optical atom chip, evanescent fields from the waveguide structure and the physics of near the surface atom-trapping will be carefully modeled. We will carry out investigations in microfabrication to ensure that the waveguide can handle required optical power and generate clean evanescent fields. For efficient atom loading, we plan to produce a constantly cooled atomic ensemble at the small-scaled waveguide location. We will also study the effect of neutral-atom adsorption on the waveguide, which may significantly modify the atom trapping potentials. Following the demonstration of trapping atoms at the waveguide and the strong photon-atom interaction, as a first high consequence application of the optical atom chip, we plan to demonstrate spin squeezing on chip for magnetometry beyond the classical limit by incorporating additional microfabricated structures. We anticipate this project will bring significant impacts to the field of neutral-atom quantum controls.

## Band Structure Engineering for Inherent Rad Hard Devices

191209 | Year 1 of 1 | Principal Investigator: G. A. Vawter

### Project Purpose:

Transient radiation effects in semiconductors can interrupt, even damage, system components. For very high photon energies associated with gamma rays and x-rays, high concentrations of electrons and holes are generated uniformly throughout the device. This mobile charge can diffuse to junctions disabling device operation. A common approach for mitigating this effect is to reduce and isolate the semiconducting volume of the device as much as practical, limiting the total charge generated that can contribute to current flow. These methods do not, however, remove or control charge generated within critical device regions.

This project investigated a new approach of band-structure engineering to control excess carriers in semiconductor devices. When combined with volume minimization via etching and substrate removal, band-structure engineering has the potential to control uncontrolled gamma-generated current within layers. The approach is applicable to pn-diodes and devices constructed from them, like bipolar transistors and even heterojunction field effect transistors. This project explores the concept of band-structure engineering for carrier control and develops simulations of AlGaAs/GaAs pin diodes quantifying the benefits as compared to conventional diodes.





## Beyond Graphene: BN-Based Semiconductor Alloys for Next-Generation Optoelectronics

180920 | Year 2 of 3 | Principal Investigator: A. A. Allerman

### Project Purpose:

Efficient UV-emitters and photodetectors enable key mission applications ranging from fluorescence-based bioagent sensing to covert, solar-blind, non-line-of-sight communications. Significant efforts worldwide have developed AlGa<sub>N</sub> alloys for UV optoelectronics, however fundamental materials challenges have precluded high-performing devices. Remaining issues include insufficient p-type doping due to fundamentally high acceptor activation energies. Hexagonal boron nitride (hBN), known as a substrate for high-mobility graphene, has recently emerged as a highly promising UV material, possessing a large bandgap of ~6eV yet remarkably showing effective p-type doping ( $>10^{18} \text{ cm}^{-3}$ ). Recent studies of hBN epilayers grown by MOVPE (metalorganic vapor phase epitaxy) report higher photoluminescence yield (~500x) and absorption (3x) than AlN, and display extraordinarily high exciton binding energy ( $>20 \times \text{GaN}$ ), portending efficient UV-emission and novel excitonic phenomena. These properties are traced to the layered crystal structure, similar to graphite, and related 2D enhancement. We propose to explore and exploit novel properties of hBN to enable next generation UV-LEDs and photodetectors. First, we will apply our in-depth experience in III-nitride material growth to extend beyond hBN to hB(Al,Ga)N alloys, achieving heterostructures for high-performance optoelectronic devices for the first time. Second, we will leverage our atomic-layer growth control to explore the potential for hB(Al,Ga)N heterostructures employing monolayer constituents. Analogous to graphene and van der Waals heterostructures, we anticipate devices with highly tailorable properties yet fabricated with modern semiconductor technology rather than layer-transfer methods. The fusion of 2D crystal properties and UV semiconductors may enable compact, robust bioagent and neutron detectors, and other novel devices relevant to NNSA and DoD applications.

## Beyond Moore's Law Through 3D-IC Fabrication

173129 | Year 3 of 3 | Principal Investigator: D. B. Burckel

### Project Purpose:

The goal of the research is to develop 3D integrated circuits (3D-ICs) at both the device and system levels. Today's ICs are fabricated using top down techniques on planar surfaces. Scaling areal transistor density has continued to increase IC performance, but requires increasingly expensive lithography equipment. Recently, we invented and demonstrated membrane projection lithography (MPL), a microfabrication technique where directional deposition through a suspended, patterned membrane was used to create micron-scale 3D metamaterials. By generalizing this fabrication approach to include patterned etch and patterned ion implantation, combined with blanket processes such as oxidation, chemical vapor deposition (CVD) deposition and planarization, we will provide a first-of-its-kind approach to 3D-IC fabrication.

Creation of 3D circuits will transform devices, systems, and technologies. For devices, fabrication in 3D enables higher transistor packing density, new geometries for devices such as power metal-oxide-semiconductor field-effect transistors (MOSFETs), and the possibility of making radiation hardened complementary metal-oxide-semiconductor (CMOS) on nonsilicon on insulator (SOI) substrates. For systems, 3D-ICs will be more difficult to reverse engineer while providing new topologies for interconnect/signal routing, improving signal integrity, and RC delay. For the first time, hybrid technologies where biological cells or photons are interfaced directly to CMOS control/sensing electronics will be possible with a mature 3D-IC platform. In order to realize these benefits, we need an entirely new fabrication paradigm capable of creating complex 3D structures in a sub-micron CMOS compatible platform and addressing issues of thermal budget, device isolation, interconnect strategies, and 3D topography-induced stress.



## Chemical Vapor into Liquid (CViL) Encapsulation of Microorganisms for Hazardous Agent Detection

173339 | Year 3 of 3 | Principal Investigator: J. C. Harper

### Project Purpose:

To detect chemical and biological threats both on and off the battlefield, development of portable, robust detection systems capable of real-time identification of these threats is essential. Living cell-based sensors have proven effective as sensitive and specific detectors, capable of near real-time detection. However, living cell-based sensors require frequent replenishment with new cells due to cellular sensitivity to the *ex vivo* environment. For cell-based devices to be practical, cells can be encapsulated in a biocompatible matrix that protects cells from environmental stresses while maintaining biological sensing functions and allowing cell-environment interaction. Silica materials have shown promise as bioencapsulation matrices due to their biological inertness, mechanical stability, simple room temperature processing, and tunable material and chemical properties. However, traditional aqueous sol-gel routes are cytotoxic to cells, limiting their use for cell-based biosensor design.

We propose, in collaboration with New Mexico Tech, to encapsulate and stabilize genetically engineered *S. cerevisiae*, *E. coli*, and *B lymphocyte* cells in porous, nanostructured silica matrices to serve as model biosensing components. Our approach utilizes a novel sol-generating chemical vapor into liquid (SG-CViL) process. This process minimizes cell contact with cytotoxic reaction constituents, allows precise control of reaction parameters, and facilitates incorporation of functional components, such as polyethylene glycol, that enhance silica gel biocompatibility. These factors make SG-CViL attractive as an encapsulation strategy for living cell-based biosensor design. This work focuses on characterizing cell-silica biocomposites, understanding the mechanism of SG-CViL-based cellular integration, assessing encapsulated cell activity, and optimizing cell-silica biocomposites for particular biosensing functions. Successful development of SG-CViL for cell encapsulation will be a significant step in designing biosensors that use living cells as the sensing unit, potentially leading to devices capable of detecting multiple threats at very low concentrations in real time.

## Developing a Solid State Technology for Electron Spin Qubits on Liquid Helium

191210 | Year 1 of 3 | Principal Investigator: E. A. Shaner

### Project Purpose:

We propose to develop electron spin qubits and the foundations of a silicon integrated circuit based quantum computing technology by integrating electrons on helium (eons) with complementary metal-oxide-semiconductor (CMOS) structures and demonstrating spin-to-charge conversion for single spin readout.

A vacuum is the best possible environment for a spin-based qubit. The eon platform embodies this ideal scenario by controllably trapping electrons in a vacuum adjacent to superfluid liquid helium. Electrons trapped in this manner represent the highest mobility 2D electron system known ( $10^8 \text{ cm}^2/\text{Vs}$ ). Microchannels on a CMOS chip stabilize the helium through strong capillary forces that make the devices insensitive to physical orientation or vibration. A truly exciting prospect for electrons on helium is that the enabling electrode chips are made using a standard silicon CMOS metallization (no modifications to materials) and even mobile eons are predicted to have coherence times of seconds or greater. The eon qubit density can be exceptionally high ( $\sim 1$  qubit per  $10 \text{ } \mu\text{m}^2$ ), eon qubits require only electrical control (no lasers or radio frequency (RF) required for confinement), and eons can be shuttled in an analogous fashion to ions in surface traps. The potential use of exchange gates in eon systems can also permit two-qubit gate operations on microsecond or shorter timescales (a requirement for realistic machines). Despite all of these benefits, the eon platform currently lacks the spin-to-charge demonstration that is required to perform any qubit operations. We will implement a Pauli blockade scheme to achieve spin readout and experimentally verify predicted spin relaxation times.

There are a handful of favored qubit approaches, including superconductors, ions, and solid state platforms. Competing approaches must have the potential to scale and perform operations at sufficient speeds for realistic operation. The 'electrons on helium' qubit platform has many compelling attributes, but lacks demonstration of spin readout or gate operations making it high risk in its current state.



## Electrochemical Detection of Single Molecules in Nanogap Electrode Fluidic Devices

180907 | Year 2 of 3 | Principal Investigator: R. Polsky

### Project Purpose:

The purpose of this project is to gain fundamental understandings of molecular diffusion in nanogap electrodes and the diffusive behavior of single molecules undergoing electron transfer. The molecules studied here are commonly used as detection tags for biological labeling. Therefore, electrochemical detection of single molecules undergoing redox cycling would enable detection of single enzymes, proteins, and DNA strands resulting in new and improved ultrasensitive sensing devices to benefit the biosecurity missions of the Department of Homeland Security and DoD. We propose to integrate orthogonal validation techniques, total internal reflection fluorescence microscopy (TIRF), and molecular simulation to clarify: 1) the mechanism leading to current build-up due to redox cycling and 2) diffusion and adsorption of single molecules undergoing redox reactions. This project leverages key Sandia capabilities: 1) Microsystems and Engineering Sciences Applications (MESA) Facility to fabricate large-area nanogaps and create nanogap electrode fluidic designs, 2) TIRF expertise to simultaneously electrically and optically monitor a molecule undergoing redox reactions unequivocally confirming that a single molecule is being measured, and 3) standard molecular dynamic simulations to determine diffusion behavior while *ab initio* molecular dynamic simulations can interrogate electron transfer as a function of electrode material. Such orthogonal monitoring coupled with innovative new device designs aided by atomistic simulations will provide an unprecedented insight into redox cycling mechanisms and fundamental information on the diffusive behavior of single molecules undergoing electron transfer. Results will be used to design basic research tools to study extracellular signaling, molecular-scale processes, internal dynamics, and intermolecular interactions, and ultrasensitive chem/bio sensors.

In order to understand how redox cycling can be used for single molecule detection the variability in measurements associated with the multitude of diffusion paths, the molecule can traverse in the channel, varying residence times, and electrostatic molecule-electrode interactions need to be understood. These molecules can then be used as biological tags for detection of single enzymes, proteins, and DNA.

## Ferroelectric Tunnel Junctions: A Physics-Based Solution to Reliable Resistive Memory

191197 | Year 1 of 2 | Principal Investigator: J. Ihlefeld

### Project Purpose:

The scientific and technical challenges to be addressed in this project are to create a reliable, reproducible, and scalable resistive memory in a 3D integratable embodiment utilizing a fab-compatible, polycrystalline ferroelectric. Success will enable broad usage of resistive memory for a range of Sandia applications, including nonvolatile memory and neuromorphic computing. Our solution utilizes a ferroelectric tunnel junction (FTJ) where the ferroelectric polarization states set the resistive state of the element. Device resistance is determined by the quantum tunneling probability through the film, and therefore, has a foundational physical principle dictating operation. Prior FTJ studies have utilized single crystalline ferroelectrics, which significantly limits scaling to wafer-scale levels. Recently, ferroelectric response in atomic layer deposited (ALD) doped, polycrystalline,  $\text{HfO}_2$  was discovered with high polarization values at thicknesses where conventional ferroelectrics display polarization reduction. ALD processing ensures uniform thin layer preparation necessary for device-to-device uniformity. Metallic and semiconducting electrodes with different work functions combined with the ferroelectric polarization-tunable barriers will be used to achieve differential resistance states. This approach is highly scalable by combining a conformally deposited polycrystalline ferroelectric film and a fundamental physics-based resistive switch to achieve memristor functionality. Systemic device-to-device variability in conventional memristors, where stochastic soft dielectric breakdown defines the memristive behavior, will be overcome. Additionally, the conformal polycrystalline film overcomes the necessity of epitaxial ferroelectrics requiring expensive single-crystalline oxide substrates that limit FTJ scalability. New science associated with polycrystalline FTJs will be developed and this project will result in the first highly scalable physics-based resistive memory element.

Memristor technology is plagued by device-to-device variability preventing broad scale implementation. FTJs are a potential solution but are a nascent technology with limited application space owing to necessary substrates and growth conditions. This project presents a heretofore-unrealized means to overcome these barriers and will provide a new capability for many national security applications by addressing these fundamental scaling challenges.



## Fundamental Scaling of Microplasmas and Tunable UV Light Generation

173131 | Year 3 of 3 | Principal Investigator: R. P. Manginell

### Project Purpose:

The purpose of this project was to build fundamental understanding of microplasma devices (MD), their scaling into the microdomain, and their ultraviolet (UV) emission physics. We hypothesized that the UV emission spectrum of MD can be manipulated real-time (sub-millisecond timescale). Applications of modulated UV emission from MD include tunable probing of quantum systems, such as atomic clock transitions, and selective chemical sensing.

We studied the temporal evolution of spectral lines from MD for the first time, including transitions to impurity states, which are prevalent in practical applications. By varying driving conditions, we can restrict deep UV emissions. This then allows for on-the-fly tuning of the ionization energy of a microplasma photo-ionization source. This is useful in chemical detection for selecting which chemicals are ionized. In atomic physics, this can be used to probe deep UV transitions with selectivity.

In order to understand the physics of MD, we developed the first fully kinetic 3D model with trends matching experiment. Using kinetic methods, we explicitly calculated the electron energy distribution function, which is significant because it is non-Maxwellian with high energy components reaching 20 eV.

This work provides fundamental understanding of microplasma devices from an experimental and modeling perspective. We developed several first-time achievements—such as real-time UV control and a fully kinetic plasma model. We developed new capabilities at Sandia for fast, deep UV spectroscopy and MD fabrication/production. This work will benefit basic science and potential applications of microplasmas including pressure sensing, chemical sensing, atomic physics, and quantum physics of interest to Sandia's national security missions.

## Highly Efficient Solar-Blind Single Photon Detectors

191199 | Year 1 of 3 | Principal Investigator: A. Armstrong

### Project Purpose:

National security applications require high sensitivity ultraviolet (UV) photodetection in the solar-blind (<280 nm) spectrum. For example, non-line-of-sight communication and Raman-based bioagent identification require near-single-photon-level detection to achieve high data rates and long range sensing, respectively. Commercial technologies including avalanche photodiodes (APDs) and photomultiplier (PMT) tubes suffer low (<10%) single photon detection efficiency and undesirable features such as cryogenic cooling, fragility, and high voltage operation.

We propose to demonstrate the first AlGaIn-based quantum dot (QD) floating gate (FG) high electron mobility transistors (HEMTs) for solar-blind detection with >40% single photon detection efficiency. Low voltage and 297 K operation of AlGaIn FG-HEMT photodetectors simplifies systems integration compared to high voltage and cryogenic commercial options. FG-HEMT photodetectors have been demonstrated for infrared (IR) photon counting. We propose to extend this proven concept to the UV-C (100-280 nm) region for the first time. AlGaIn FG-HEMT photodetectors can achieve high single photon detection efficiency at >297 K through extreme QD/matrix energy contrast to localize photogenerated carriers between the channel and gate. A single QD-trapped carrier changes the gate-drain bias, which is amplified by the large transconductance to produce a measurable current transient. Low dark count rates and high frequency response, which are critical for threat detection and communication, are anticipated compared to APDs because the photoconductive gain does not require the device to be operated near electrical breakdown or recover from avalanche.



## Magnetic Josephson Junction Memory and 3D Integration for Scalable, High Performance, Low Power Computing

180906 | Year 2 of 3 | Principal Investigator: N. A. Missert

### Project Purpose:

Superconducting electronics (SCE) is one of the leading technology candidates for high performance, ultralow power computation needed by Sandia's national security sponsors. Although high-speed, digital superconducting circuits have been demonstrated, the promise of extending these devices to high performance computing has been severely hindered by the lack of a fast, low energy, high capacity, integrated memory cell, and scalable 3D active device structure. This project addresses each of these issues by employing novel, tailored, ferromagnetic thin films for memory cells integrated with a Josephson junction (JJ) structure that can be fabricated in 3D by using an alternative superconducting layered system. In contrast to the Nb/AlO<sub>x</sub>/Nb JJ technology currently employed for SCE, where degradation issues do not allow 3D stacking of the active JJ layers, our approach exploits the relative stability of niobium and tantalum nitrides for the logic gates and chromium-doped aluminum and gallium nitrides for ferromagnetic memory elements. The technical challenges include understanding and optimizing Cooper-pair transport across both the TaN layer near the metal-insulator transition and the single-domain Cr:AlN and Cr:GaN soft ferromagnetic layers, as well as ultimately demonstrating an integrated working memory cell in a 3D stack. If successful, this work will provide the foundation for the next generation of truly scalable SCE for high performance, low power computing.

## Optimization of Sputtered Aluminum Nitride for the Seeding of MOCVD Gallium Nitride Films

191204 | Year 1 of 3 | Principal Investigator: K. Knisely

### Project Purpose:

The goal of this project is to develop Gallium Nitride (GaN) on silicon (Si) capabilities in Sandia's Microsystems and Engineering Sciences Application (MESA) fabrication facility. GaN on Si combines the electrical benefits of GaN (high current levels, high breakdown voltage, long device lifetimes) with the cost and scaling benefits of Si processing techniques used by the complementary metal-oxide-semiconductor (CMOS) industry. GaN growth on Si wafers is difficult to achieve, because it requires a highly oriented buffer layer that can properly orient the III-V film on lattice mismatched substrates such as Si. Sputtered aluminum nitride (AlN) is an attractive buffer layer material, as it is a scalable, CMOS compatible, and has been demonstrated to seed high quality metal-organic chemical vapour deposition (MOCVD) GaN films on sapphire substrates. This project leverages the existing exceptional III-V, CMOS, and sputtered AlN capabilities at MESA Fab to explore and characterize the material science governing MOCVD film growth on Si substrates using sputtered AlN as a seed layer, ultimately benefitting applications such as LEDs, MEMS, and power electronics. This is achieved by characterizing how factors such as AlN grain size, stress, thickness, and the underlying substrate material properties affect the MOCVD films' growth behavior. MOCVD film performance will be quantified using precision metrology (x-ray diffraction [XRD]), photoluminescence, and scanning transmission electron microscopy (STEM) and radio frequency (RF) resonator device performance comparisons, with the goal of developing III-V films grown on Si that have comparable quality to films presently grown on sapphire, using MOCVD nucleation layers, at MESA Fab.





## Piezoelectric Nano-Optomechanical Systems

173496 | Year 3 of 3 | Principal Investigator: M. Eichenfield

### Project Purpose:

The field of nano-optomechanical systems (NOMS) investigates photon-phonon interactions in nanoscale volumes. Optomechanical crystals (OMCs) are metamaterials that allow photons and phonons to be confined within a nanoscale volume for strong interactions. OMCs have been used to test quantum limits and study the quantum effects in mechanical systems due to their exquisite sensitivities to motion. However, many ground-breaking applications of these systems are still outstanding.

An area that just beginning to be explored in this field are photon-phonon-charge interactions in NOMS using optically transparent piezoelectric materials, such as aluminum nitride and lithium niobate. Previous devices were fabricated using silicon and silicon nitride, which are not piezoelectric. However, Sandia has developed new capabilities in the micromachining of piezoelectric thin films, and these capabilities could and should be used to study optomechanics in piezoelectrics.

In addition to standard photon-phonon interactions, piezoelectric NOMS include electromechanical piezoelectric interactions, essentially coupling the internal charge distribution of the material to the light and mechanical vibrations. The dynamics of these systems are unexplored and offer myriad possibilities for study of their fundamental properties and potential applications.

Creating piezoelectric NOMS devices is a worthwhile goal, but it is also challenging. To make these devices, one needs to precisely fabricate nanoscale systems in materials like lithium niobate and aluminum nitride, which are difficult to fabricate and still experimental compared to standard complementary metal-oxide-semiconductor (CMOS) materials. Moreover, there are theoretical, numerical, and experimental challenges to solve to design and test such devices.

To successfully create piezoelectric nano-optomechanical systems, with large optomechanical and piezoelectric coupling to structural vibrations, we must leverage very recent advances in disparate fields: ultra-thin-film electromechanical devices, nanofabrication of piezoelectric materials, piezoelectric photonics, and RF acoustics.

This work is in collaboration with the University of New Mexico.

## Reduced Dimensionality Lithium Niobate Microsystems

173126 | Year 3 of 3 | Principal Investigator: M. Eichenfield

### Project Purpose:

Next-generation optical and radio frequency (RF) communications components require unprecedented bandwidth, low power, efficiency, and small size. Because of its superior piezoelectric coupling, low acoustic/optical loss, high nonlinear optical susceptibility, and optical transparency over broad wavelengths (350 to 5200 nm), lithium niobate has found widespread use in RF filters, laser frequency doublers, and acousto-optic (AO) devices. We proposed a new class of acoustic, optical, and AO devices with orders of magnitude improvements in bandwidth, power consumption, efficiency, and size enabled by reducing the dimensionality of  $\text{LiNbO}_3$  structures. By micromachining  $\text{LiNbO}_3$  into suspended structures where the thickness and in-plane features are on the order of, or much smaller than, the acoustic/optical wavelength, the already outstanding piezoelectric and optical properties of  $\text{LiNbO}_3$  can be significantly enhanced—with corresponding improvements in device performance. We proposed to demonstrate these theoretical performance benefits in a novel AO modulator. Several scientific and technical problems must be solved including the realization of suspended  $\text{LiNbO}_3$  structures with the desired small features, optical and acoustic properties and the modeling and co-design of AO structures in strongly anisotropic materials.

We showed, for the first time, a completely on-chip approach to frequency doubling with low optical powers (milliwatts). This is important for on-chip synthesis of optical clocks, where it is necessary to double individual frequency comb lines. We also demonstrated high generation rates of entangled photon pairs in an on-chip system, which is necessary for many quantum communication protocols that are currently being pushed into on-chip platforms. Finally, we demonstrated low-voltage, low-power amplitude and phase modulation on-chip, which are important for telecommunications and many other optical applications on-chip.



## Scandium Aluminum Nitride for Advanced Piezoelectric Sensors, Actuators, and Filters

191198 | Year 1 of 3 | Principal Investigator: B. Griffin

### Project Purpose:

The project's purpose is to fundamentally understand effects of alloying of nitride piezoelectrics leading to revolutionary filters, sensors, and actuators. The current market for wireless radio frequency (RF) filters for cellular is dominated by aluminum nitride (AlN) piezoelectric resonators, specifically film bulk acoustic resonators (FBARs). FBAR success is due to superior combination of bandwidth, out-of-band rejection, insertion loss, and complementary metal oxide semiconductor (CMOS) compatibility. The maximum bandwidth achieved by these filters is half the material-limited electromechanical coupling coefficient ( $k^2/2=3\%$ ). However, FBARs are half-wavelength, thickness mode resonators fundamentally constrained to a single frequency per chip.

Lamb-wave mode resonators overcome this limitation by achieving resonance in the plane of the film, where frequency is established by lithography rather than film thickness. Sandia's microresonator program demonstrated this advantage with 32 kHz to 10 GHz resonators on a single chip. Although microresonators have tremendous potential, they cannot meet the bandwidth requirements for many current RF needs because of the AlN's low lateral coupling coefficient ( $k^2/2=1\%$ ). Recent research suggests that an alloying level of 41% scandium increases  $k^2/2$  to 15%. An improvement of 1/5th this value would enable breakthrough radio designs using single chip, multifrequency filters. However, research to this point has focused on material development. We will study the effects of scandium alloying of AlN for device performance to enable mass adoption of Sandia's microresonator technology. Advancements in this area will also enable a new class of microscale piezoelectric sensors and actuators.

The goal of this effort is to understand the effects of scandium alloying levels on piezoelectric nitride based devices. We propose to achieve this through careful measurements of film properties and ScAlN-based device platforms. Success is defined as developing an understanding of the new design space enabled by scandium alloying.

## The Anatomy of the Minority Carrier - Atomic Cluster Interaction in Semiconductors

173127 | Year 3 of 3 | Principal Investigator: B. L. Doyle

### Project Purpose:

The purpose of this project is to use light ion beam induced charge (IBIC) to detect damage cascades generated by a single heavy ion, and thereby reveal details of the shape of the cascade and the physics of recombination of carriers that interact with the cluster. IBIC measurements of damage cascades will improve the accuracy of theoretical models used to predict electrical degradation in devices exposed to radiation environments. In addition, light ion IBIC detection of single ion-induced damage could be used to locate single ion implantation sites in quantum computing applications. This project uses Sandia's unique nanolimplanter (nl) technology to produce heavy ion-induced collision cascades in p-n diodes, simulating cascades made by primary knock-on atoms. The nl is also used to perform highly focused scans that generate IBIC signals. The IBIC signal produced by each light ion maps regions of lower charge collection efficiency without incurring further damage.

Thermonuclear detonations produce high energy fusion and fission neutrons that cause degradation of electrical performance in semiconductor devices used in weapon circuits. In this project, we used IBIC to examine the influence of these collision cascades on carrier recombination produced by high-energy single heavy ions. The system developed "NanoBeam Channeled" IBIC (NBC-IBIC) represents the first light-ion, nano-focused, ion-channeling, IBIC system in the world. NBC-IBIC will find many applications to future programs at Sandia including improving the understanding/quantifying Shockley-Read-Hall electron-hole recombination in the vicinity of electrically active defect clusters.



## Vertically-Injected Ultraviolet Laser Diodes

188288 | Year 2 of 3 | Principal Investigator: M. H. Crawford

### Project Purpose:

Extension of laser diodes (LDs) throughout the ultraviolet (UV) spectral region is thus far unrealized but would be a significant technological breakthrough. Such compact, rad-hard lasers are of interest for fluorescence-based bioagent sensing, trapped-ion quantum computing and technologies in the solar-blind region ( $< 280$  nm). To date, however, milliwatt (mW) class UV LDs are limited to pulsed operation at longer wavelengths ( $> 335$  nm) due to materials challenges of AlGaIn wide-bandgap semiconductors. One major roadblock is the lack of an electrically conductive, lattice-matched substrate, yielding non-radiative defects and forcing lateral-injection designs that limit performance by current crowding and heating. A second roadblock is the deep acceptor levels that preclude thermal activation of holes needed for effective p-type doping. Finally, little is known about the dominant contributions to optical loss in these laser structures, frustrating device design optimization. To overcome these challenges, we propose to explore three primary thrusts. First, we will move beyond sapphire substrates to develop templates based on micro-patterned bulk GaN substrates. This approach will simultaneously achieve benefits of vertical-injection laser designs, crystallographically cleaved facets, and reduced threading-defect densities. We will then apply these lasers to quantify contributions of p-type doping to optical loss in UV AlGaIn lasers for the first time. We will further explore the potential for Mg-doped superlattices to enable polarization-field-based activation of holes for enhanced p-type doping. Our overall goal is to apply these advances to demonstrate lasers at  $< 335$  nm, thereby achieving the shortest wavelength mW-class LDs to date.

This project is cutting-edge research with potential to advance the state of the art in UV LD performance. The work is high risk, given the formidable materials challenges of wide-bandgap semiconductors and proposed innovative approaches that have not been previously realized for UV LDs.

## Understanding the Physics of SiGe HBTs for Cutting-edge Electronics at Deep Cryogenic Temperatures

193422 | Year 1 of 3 | Principal Investigator: T. D. England

### Project Purpose:

Sandia applications in sensing, quantum computing, and space-based systems often require deep cryogenic temperature operation where many electronics fail. Prior work has shown that silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs) actually improve as they are cooled to cryogenic temperatures. Unfortunately, previous research down to 4 K has been limited and left a number of questions about the physics of transport in these devices. The purpose of this project is to discover new device physics and leverage that knowledge to create cutting-edge analog and radio frequency (RF) circuits with SiGe HBTs operating at 4 K.

The first phase of this project is a discovery phase in which new understanding will be created by the study of the physics of transport in SiGe HBTs at 4 K. The Georgia Institute of Technology team will study the impact of multiple scaling generations, complementary devices (negative, positive, negative [NPN] and positive, negative, positive [PNP]), and more than one commercial foundry on the performance of SiGe HBTs at 4 K. The second phase will begin the creation of high-performance analog electronics, leveraging the understanding from phase 1 to take full advantage of SiGe HBT technology to design and measure the analog electronics at 4 K. Phase 3 will include the development of additional high-speed analog and RF circuits, and design of a high-frequency amplifier. Amplifiers of this type can greatly aid sensor readout and communications at 4 K.

The circuits will have the potential to quickly impact applications and place Sandia at the forefront of 4 K electronics. The process of creating the circuits will result in the development of a circuit design methodology with SiGe HBTs at 4 K that has the potential to streamline the creation of an entire suite of game-changing electronics.



## Visible Quantum Nanophotonics

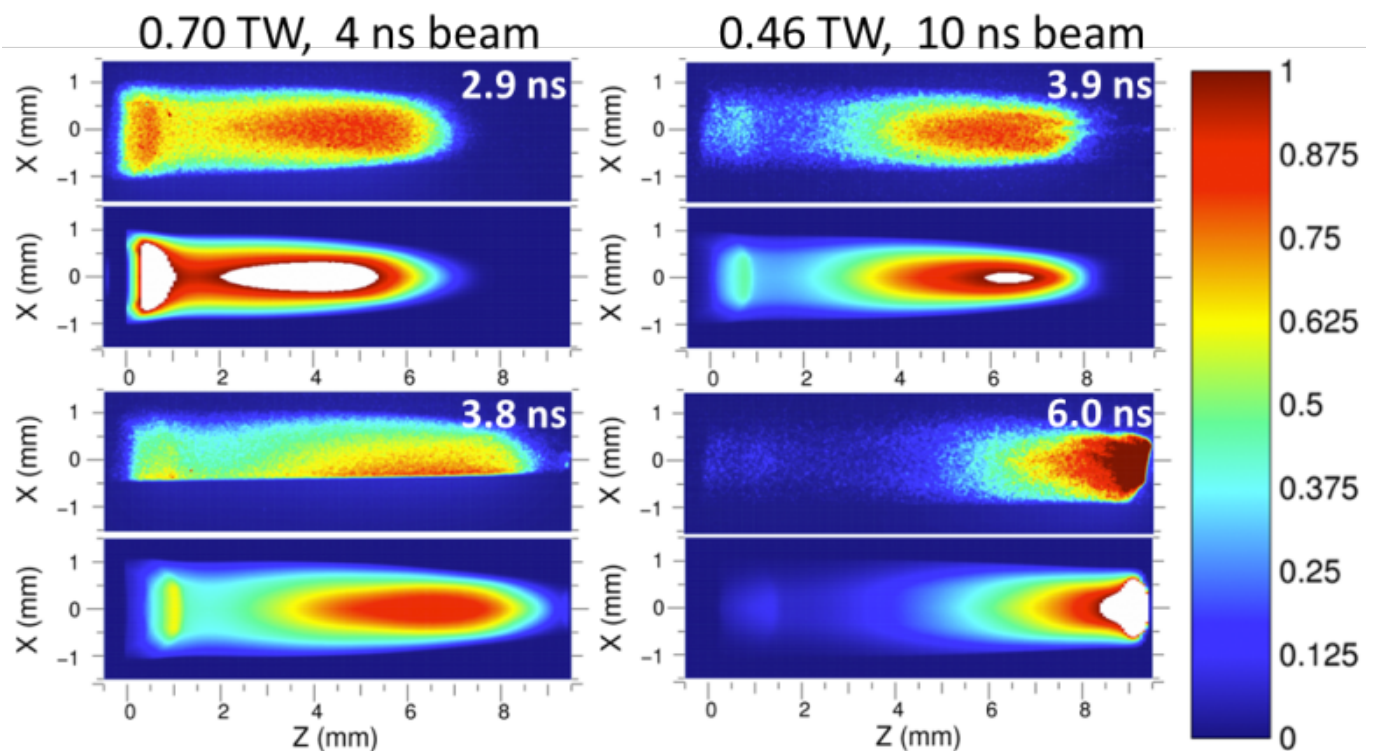
186113 | Year 2 of 3 | Principal Investigator: G. S. Subramania

### Project Purpose:

Applications for ultraviolet/visible lasers are many and include: free-space and underwater communications; solid-state lighting; biosensing/actuation/cide; free-space directed energy; quantum communication; and atomic clocks. All of these applications will benefit greatly from improvements in two key characteristics: electrical-to-optical energy-conversion efficiency, and directability. At one extreme, low-power applications need maximum useful work for minimum energy consumption; at the other extreme, high-power applications are typically heat-sink limited at the source and target-localization-limited at the sink.

The key to past improvements in efficiency and directionality has been simultaneous control over electron and photon confinement (in real space) and densities of states (in reciprocal space). Though past improvements have been revolutionary, practical devices use one-dimensional structures: quantum wells for control of electrons and Fabry-Perot-like cavities for control of photons. Even more revolutionary improvements are possible when control is extended to more than one dimension.

In this project, we propose to develop a quantum nanophotonics laser architecture in the visible that enables practical control over electrons and photons in more than one dimension. We propose to control electrons by fabricating quantum dots (QDs) with precision spatial and spectral control. Photons will be controlled using photonic crystals and specifically, we propose to investigate photonic-crystal surface-emitting laser (PCSEL) architectures, again with precision spatial and spectral control. Ultimately, such quantum nanophotonic QD-PCSELs could enable: unprecedented efficiency and directability and thus wide “forward” fan-out to the applications mentioned above; and wide “backward” fan-out to science questions associated with a new and unexplored regime of mesoscale quantum optics.



## Radiation Effects and High Energy Density Sciences

The Radiation Effects and High Energy Density Sciences Investment Area seeks to advance science and engineering in the areas of radiation effects sciences, dynamic material properties, high energy density science, and pulsed power science. The goal of the radiation effects sciences area is to ensure that engineered systems are able to operate as intended in radiation environments they encounter, with a particular interest in developing pulsed power technologies, innovative experimental techniques, and novel diagnostics that could scale to higher energy drivers.

*The image above shows comparison of time-gated self emission between experiments (top) and simulations (bottom) for laser beams depositing energy into pure Ar gas at different times. The excellent agreement suggests codes can model Magnetized Liner Inertial Fusion preheat. (Project 173190, Investigating Laser Preheat and Applied Magnetic Fields Relevant to the MagLIF Fusion Scheme)*

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## An ion-Neutron Electron-Gamma SIMulation System for Radiation Testing of Optical Components for Weapons Systems - NGOSIM

173192 | Year 3 of 3 | Principal Investigator: B. L. Doyle

### Project Purpose:

The purpose of this project is to modify a previously developed Neutron-Gamma irradiation SIMulation (NGSIM) system (used to test electronics) to enable testing of optical (NGOSIM) components. The proposed NGOSIM system would be built and operated at Sandia's Ion Beam Lab (IBL) and would simulate both neutron and gamma irradiations using <40-MeV ions and <100-keV electrons plus photons, respectively. We will add new optical input and output capabilities for simulating and measuring optical devices in both the temporal and spectral domains. The new NGOSIM capability will be applied to study the radiation effects on potential weapon components (e.g., photovoltaics, optical fibers, and solid-state laser materials) at irradiation levels comparable to historic Sandia radiation facilities: SPR-III (neutrons) and Hermes-III (gammas).

This project will establish a new first-of-its-kind experimental radiation simulation capability that goes beyond historic radiation facilities in certain respects: the ability to independently control displacement damage and ionization, for variable exposure times (from nanoseconds to seconds), and to change flux values quickly over a large dynamic range. These new experimental capabilities will enable a better understanding of the dynamics of radiation-induced defects in optical materials, thereby improving radiation tolerance of future optically based weapon components. Early in the design and development of weapon optical components, NGOSIM experiments will result in the selection of materials that degrade the least when exposed to hostile radiation. This will not only speed the realization of optical components for weapons, but also reduce costs considerably.

## Application of Enhanced Photocurrent Models and Single Event Effects

181198 | Year 2 of 3 | Principal Investigator: D. A. Black

### Project Purpose:

This project explores the capabilities and limitations of several analytic photocurrent models for application to dose rate effects in CMOS7 (complementary metal-oxide-semiconductor) devices and circuits. Understanding the effects of photocurrent in stockpile circuits and application specific integrated circuits (ASICs) is critical for characterizing weapon performance in hostile environments. Circuit simulation plays an important role in enhancing that understanding. However, a thorough comparison of the various compact model approaches, with an understanding of their physics, capabilities and limitations, has not been comprehensively documented.

This project goes beyond standard model development and calibration efforts and will create a comparative understanding of the physics of the various compact models. The effort will create bounds on the models for the various technologies and drive future compact model development.



## Cavity Electron Density Measurements within Pulsed Radiation Environments

177967 | Year 3 of 3 | Principal Investigator: K. S. Bell

### Project Purpose:

This project aimed to address the need to understand the plasma characteristics within a systems-generated electromagnetic pulse (SGEMP) cavity and how we can make measurements of the system for code validation. The primary measurements within these cavities provide information on the currents without information on the plasma conditions. To further the understanding of the plasma conditions, this project's goal was to develop a fiber optic interferometer tailored to the simulated environment to measure chordal electron density within the cavity in difficult to access configurations in high radiation environment produced by the Z machine.

In this project, a fiber optic diagnostic using 1550 nanometer light and based on photonic displacement interferometry was built and characterized. This diagnostic can probe low density plasmas in difficult to access configurations in high radiation environment produced by the Z machine. Improvements to design and fielding methodology over the development of the project allowed for minimal background from radiation-induced phase change using standard single mode fiber. This allows for high quality measurements without the need for radiation-hard fibers which can be difficult to obtain or prohibitively expensive. By the completion of the project, an additional diagnostic for use within SGEMP cavities was created that will allow for improved understanding of the system and significantly increase the number of experimental quantities available for code validation.

The results of this project will provide data for validation of radiation and plasma models used for NNSA and DoD sponsors that are concerned about radiation effects science.

## Compact Models for Defect Diffusivity in Semiconductor Alloys

180932 | Year 2 of 3 | Principal Investigator: A. F. Wright

### Project Purpose:

Predicting the transient effects of short-pulse radiation in semiconductor devices is an important activity for Sandia's national security missions. Recently, the material of choice for radiation-tolerant semiconductor devices shifted from silicon to III-V compounds such as GaAs. One benefit of this shift is that it enables engineers to use alloys such as InGaAs to optimize the radiation tolerance of a given device. However, the computer codes currently used to model transient effects will need to be modified because they assume that pertinent point-defect characteristics, such as their diffusivities, do not change with time. This is true in a binary compound such as GaAs, but not in an alloy such as InGaAs because the characteristics of a defect depend on the types of atoms near it and, therefore, on its location in the alloy. Specifically, irradiation initially creates defects at random locations in the alloy, but their local environments—and hence their characteristics—can change as they migrate through the alloy. To include these changes when modeling transient effects, we are using results from density functional theory (DFT) and kinetic Monte Carlo (KMC) simulations to develop compact models that accurately model the time dependence of pertinent defect characteristics. Specifically, DFT is being used to calculate stable-state and saddle-point energies at a set of locations in a random alloy, and these energies are then used to develop cluster expansions from which we obtain these energies at arbitrary locations in the alloy for use in KMC simulations of defect migration.



## Correlating the Structural and Electrical Performance of Microelectronics during a Radiation Event

191240 | Year 1 of 3 | Principal Investigator: K. M. Hattar

### Project Purpose:

Radiation-induced displacement damage is an issue for materials used in many applications including nuclear reactors, space electronics, and nuclear weapons microelectronics. Disruption of the crystalline structure due to displacement damage and its evolution in time can alter the structure, band gap, and electrical properties of these materials. After the cascade is done (picoseconds), the resulting defects will diffuse and interact over timescales from nanoseconds to the life time of the device, affecting the material properties and reliability. However, a direct correlation between the discrete and stochastic nature of radiation damage and the resulting change in properties at the device level remains challenging due to constraints associated with the experimental techniques and modeling methodologies that are currently available.

We propose an approach that will provide fundamental understanding of the initial creation, fast reaction, and long-term evolution of collision cascades in materials. The unique capabilities of the in situ ion irradiation transmission electron microscopy (I<sup>3</sup>TEM) at Sandia will be utilized to directly observe displacement damage due to single ion events at near atomic resolution. In addition, the I<sup>3</sup>TEM capabilities will be expanded to cover the important temporal scales ranging from nanoseconds to hours. We will also combine modern TEM image analysis models with defect recombination models to explain the time evolution of the damage cascades. If this experimental advancement and computational coupling is successful, it will provide a unique tool set to address materials' responses in a range of complex extreme environments.

These research findings will provide needed fundamental insights into irradiation-induced defects evolution at a length scale and time resolution not previously accessible experimentally, as well as a coupled modeling approach. The results would provide calibrated input into current continuum models used to predict microelectronics response to hostile threat environments.

## Coupled Electron-Photon Monte Carlo Radiation Transport for Next-Generation Computing Systems

195880 | Year 1 of 3 | Principal Investigator: K. Bossler

### Project Purpose:

Exascale supercomputers will likely consist of heterogeneous architectures, combining multicore central processing units (CPUs) with either graphics processing units (GPUs) and/or many integrated core (MIC) coprocessors. Top supercomputers increasingly rely on GPUs and MICs because they offer high computing power and energy efficiency through a single instruction, multiple data (SIMD) paradigm.

Traditional Monte Carlo radiation transport codes rely heavily on algorithms that are inherently divergent and memory-intensive due to the stochastic nature of the "history-based" particle tracking process. The divergence problem is exacerbated further in coupled electron-photon transport because both electrons and photons can be tracked within each history. For these codes to be effective on next generation computing systems, they must evolve to consider algorithms better suited to the thread-level parallelism required by the SIMD paradigm.

While some research has been done on the effectiveness of GPUs and MICs for Monte Carlo radiation transport, there are two concepts that appear to be ideal for the SIMD paradigm that have not been considered for coupled electron-photon transport. The first is post-processing particle tracks and the second is "event-based" particle tracking for both electrons and photons. This project will explore both concepts for architectures that include GPUs.

Post-processing particle tracks should help mitigate memory concerns by processing tallies separately from the transport simulation, which frees resources for other memory-intensive data such as geometry and cross sections. Three algorithms will be implemented—apportioning tracks across mesh elements using exact and approximate methods and using the kernel density estimator (KDE) method.

"Event-based" particle tracking should help mitigate divergence issues due to processing particles in groups rather than individually. This would represent a paradigm shift for production Monte Carlo codes. "Event-based" particle tracking will be implemented as part of a new code for solving coupled electron-photon transport problems using both CPUs and GPUs.



## Creating the Foundation of Next-Generation Pulsed-Power-Accelerator Technology

173191 | Year 3 of 3 | Principal Investigator: B. Stoltzfus

### Project Purpose:

We propose to create the foundation of next-generation pulsed power accelerator technology. The technology would serve as a critical milestone on the path to the development of Z 300, Z 800, Thor, Neptune, Pluto, and a next-generation multipulse radiographic linear induction accelerator (LIA).

This foundation begins with the design of a high reliability, high power density "brick." These bricks consist of two capacitors and a switch and serve as the building blocks for all of our proposed machines. Developing high reliability and high power density at the brick level directly translates to high reliability and high power density at the final machine level. For this reason, rigorous development of the brick components has a far-reaching impact on the performance of future machines. This need highlights the importance of the single-brick and Thor-1 test facilities which allow for high shot count testing and rapid prototyping to quickly evaluate high-risk, high-payoff brick modifications.

In addition to individual brick development, it is vital that we explore brick integration into formats such as linear transformer drivers (like Pluto, Z 300, and Z 800) and cable pulsers (Thor, Neptune, a multipulse LIA, and a dense plasma focus driver). Understanding the complex interaction between bricks under various conditions and scenarios is critical to understanding how the machine will perform as a whole. If a novel brick idea is successful at the single brick level, we will be able to test it at the integrated level using the new Pluto cavity or Thor-24 facility. In this effort, we are contributing to the foundation for the world's largest and most powerful pulsed power accelerator.

## Current Loss in 0.1 - 100 Terawatt Vacuum Transmission Lines: Next-Generation Experiments and Physics-Based Simulations

191237 | Year 1 of 3 | Principal Investigator: B. T. Hutsel

### Project Purpose:

A system of magnetically insulated transmission lines (MITLs) is commonly used by superpower accelerators to deliver electrical power at megavolts and mega-amperes to a physics package load. Such a system comprises a number of MITLs connected electrically in parallel by a post-hole vacuum convolute. The convolute is a complex 3D structure that serves as a current adder: it combines the currents at the outputs of the MITLs and delivers the combined current to the load.

As an MITL system is operated at increased levels of electrical power density, current losses in the system increase. Even a small loss can result in substantially reduced performance of the physics package load, since the performance can scale as strongly as  $I^4$ . Currently, such losses are not well understood. Electrical power flow at high power densities generates plasmas that evolve from MITL system electrode surfaces that are not described in traditional analytic and computational MITL models. It is currently unclear from what materials the electrodes of a MITL system should be fabricated, and how the electrodes should be fabricated, cleaned, stored, installed, and cleaned again in situ before an accelerator shot.

We propose to conduct power flow experiments on Mykonos and Z, and concurrently develop next-generation physics-based theoretical models of the experiments. Our goal is to develop predictive circuit and fully electromagnetic, fully relativistic, 3D particle-in-cell (PIC) models of a MITL system. The predictive models will be used to demonstrate that we can, with confidence, build next-generation superpower accelerators such as Z 300 and Z 800.

This project aims to understand electrical power flow in vacuum transmission lines at high power densities relevant to systems like Z. New advancements in power flow models are needed in the very near future in order to develop the predictive capabilities necessary to have a high level of confidence in the designs of future pulsed power accelerators.





## Development of a 200-kV, Low-Inductance, Low-Jitter, Low-Prefire-Rate Spark-Gap Switch

191238 | Year 1 of 2 | Principal Investigator: M. L. Wisher

### Project Purpose:

Fast, reliable switching is the basis of all pulsed power systems. The international pulsed power community has not yet developed such a switch. This is a 50-year-old problem. The community has not developed a switch design—and an associated set of fabrication, cleaning, assembly, and operating specifications—that will lead to the switch performance that will be needed by the new proposed Thor, Neptune, Pluto, Z-300, and Z-800 accelerators. This project seeks to create a prototype, easy-to-trigger, low-prefire-rate, low-inductance, high-current, high-voltage compact gas switch suitable for next-generation pulsed power accelerators.

Sandia's present baseline linear transformer driver (LTD) switch improves circuit performance, but does not provide reliable, repeatable operation due to the complexity of the switch assembly. Furthermore, a complex design is expensive in terms of fabrication and assembly time. Sandia's institutional skill in designing high-voltage, pressurized switches can accommodate the high-performance aspects of the baseline switch into a simplified package. The design created by this project will exhibit the requisite performance, while eliminating the mechanical complexities that make the present baseline design difficult and expensive. The prototype switch will meet the requirements for a next-generation linear-induction accelerator. Developing one switch that can meet the requirements for such a large number of machines will reduce the cost to develop the machines.

This effort seeks to create revolutionary pulsed power technology, and involves a substantial amount of risk to achieve the delicate balance of state-of-the-art performance and high reliability.

## Extending the Accessible Range of Strain Rates on Z using Continuously Graded-Density Flyers Fabricated using Sputter Deposition

180933 | Year 2 of 2 | Principal Investigator: D. P. Adams

### Project Purpose:

While the research of dynamic materials properties using Sandia's Z machine has been tremendously successful over the last 15 years, there are limitations. One is the range of strain rates accessible in off-Hugoniot experiments, for example, when measuring material strength at high pressures. Present experiments on Z are limited to strain rates of about  $10^5 \text{ s}^{-1}$ . Experiments at laser facilities like the National Ignition Facility (NIF) operate at much higher rates  $\sim 10^7$  to  $10^8 \text{ s}^{-1}$ , resulting in a strain-rate gap between Z and NIF. This strain-rate gap poses challenges for cross-platform validation of experimental results.

The purpose of this project is to close the strain-rate gap by developing a platform for Z ramp compression at two to three orders of magnitude faster rate than currently available. The present approach to Z ramp compression is limited in strain rate by the current pulse rise time—obtaining markedly shorter rise times is not currently possible. Instead, we explored a different approach. Our team investigated whether a thin, graded-density flyer coating provides suitable generation of high loading and unloading strain rates. The leading-edge research component of the project is the reliable production of low-stress, graded-density, impactor films with uniform thicknesses. This task was challenging because the necessary thickness is below that accessed by previous graded density fabrication methods (spray, tape casting) but well above that attained by vapor deposition techniques such as sputtering. The potential benefits of thin graded density flyers were addressed with predictive modeling of high velocity impact and validation tests on Sandia's STAR facility two-stage gas gun.

In summary, a new graded density flyer technology has enabled shock-ramp compression experiments at loading and unloading rates that are two decades greater than previous approaches on Z. The newly attained strain rates are similar to the rates provided by laser-based facilities such as NIF. This new capability should facilitate cross-platform validation experiments that determine the strength of different materials at high pressures.



## Investigating Laser Preheat and Applied Magnetic Fields Relevant to the MagLIF Fusion Scheme

173190 | Year 3 of 3 | Principal Investigator: A. B. Sefkow

### Project Purpose:

Realizing controlled thermonuclear fusion (i.e., ignition) with an inertial confinement fusion (ICF) concept is important for demonstrating our understanding of the atomic behavior at extreme conditions. Ignition has not been achieved yet due to challenging requirements for the traditional, thin-spherical-shell ICF concept. Magnetized liner inertial fusion (MagLIF) is a new economical ICF concept, where a thick cylindrical shell filled with fuel is imploded with a pulsed power driver. MagLIF has gained attention from the ICF community because its key concept—fuel-preheat and magnetization—may relax the challenging requirements. Preheating the fuel to a few hundred electron volt temperatures reduces the compression needed to heat the fuel to ignition-relevant temperatures. Fuel magnetization can improve ICF performance in two ways: 1) by suppressing thermal conduction to enhance the fuel heating efficiency and 2) by trapping charged particles to induce further fusion reactions.

Initial integrated Z MagLIF experiments in FY 2014 showed that fuel preheat and magnetization has a significant impact, but the fusion yield was lower than simulated. One hypothesis is that laser-fuel coupling was not as efficient as simulations suggest. However, to date, there have been very few experimental studies of laser heating and propagation in magnetized plasmas at conditions relevant for MagLIF to test this, because the conditions are challenging to produce and diagnose. This makes studies in this parameter space of general interest to the high energy density physics community. This project aims to investigate laser preheat and fuel magnetization by performing focused experiments at major high energy density facilities including Sandia and the Laboratory for Laser Energetics.

## Measuring Plasma Formation, Field Strength, and Current Loss in Pulsed Power Diodes

180935 | Year 2 of 3 | Principal Investigator: M. D. Johnston

### Project Purpose:

The purpose of this project is to develop diagnostic capabilities to measure current flow in high-power diodes, and in particular, the final-feed gap on Sandia's Z machine, where current losses of up to 20% occur on some loads. The project's primary focus is on measurements of load current and near-term mitigation of losses. This research, combined with high-fidelity, particle in cell (PIC) code development (EMPHASIS and LSP), is necessary to improve our physics understanding and increase the overall predictive capabilities for future, higher-current machines, such as Z-Next. This work will concentrate on the final-feed section, where only a very limited amount of data has been collected to date. Plasma formation and propagation will be studied using diagnostics, such as high resolution visible and ultraviolet spectroscopy. Spectroscopy is a powerful tool for the analysis of plasmas in pulsed power machines. Spectroscopy can provide information on the temperature, species densities, plasma velocities, and E- and B-field orientations and strengths, in a nonperturbing manner. While this project concentrates on the magnetic field, through the Zeeman effect, as a method to diagnose current flow, important data on other plasma parameters will be obtained as well. Work of this type on Z is very challenging and is the first of its kind. To help ensure the success of the Z measurements, measurements were also taken on the Self-Magnetic Pinch (SMP) e-beam diode, fielded on the Radiographic Integrated Test Stand RITS-6 accelerator. RITS offered a convenient platform, with similar high fields, but greater optical access, easier experimental planning/flexibility, and lower cost. The RITS experiments helped to guide, improve, and increase the chances for success for the shots on Z. While optical spectroscopy is a proven method, the harsh environment on Z poses many challenges. This project will provide a strong foundation to build understanding of current loss mechanisms and mitigation schemes necessary for the long-term success of future pulsed power devices.



## Modeling of Nonlocal Electron Conduction for Inertial Confinement Fusion

173868 | Year 3 of 3 | Principal Investigator: L. Lorence

### Project Purpose:

This research, in collaboration with the University of Wisconsin-Madison, will advance modeling of nonlocal electron conduction for direct drive inertial confinement fusion (ICF) target implosions. Current capability involves multi group diffusion-based theory of “diffusing” higher order moments of the electron distribution function to simulation nonlocal electron thermal conduction. In this research, a new implicit Monte Carlo—discrete diffusion Monte Carlo (IMC-DDMC) numerical algorithm—developed for x-ray transport will be used to efficiently simulate nonlocal electron conduction. The details of applying this hybrid transport-diffusion theory to electron physics with its electromagnetic fields are not obvious. However, the efficacy of the hybrid IMC-DDMC method for computationally efficient transport of x-ray photons appears promising. This study seeks to apply this advanced numerical method to electron physics. One goal is to more accurately include the effects of electric and magnetic fields in this theory. The result would be improved modeling of nonlocal electron conduction, an important ICF phenomenon for target implosions. The work will involve advanced modeling of nonlocal electron conduction in the multidimensional radiation hydrodynamics simulation code, DRACO.

DDMC is not being use in production codes as of yet; the method proposed is new and has yet to be applied to electron physics. It has the potential to allow for more accurate simulation for nonlocal electron conduction, especially those encountered in high energy density type problems where very steep temperature gradients are found.

## Optimization of Isentropic Compression Loads on Current-Adder Pulsed Power Accelerator Architectures

181063 | Year 2 of 2 | Principal Investigator: D. Reisman

### Project Purpose:

The magnetically driven isentropic compression technique (ICE) was originally developed on the ZR accelerator. It has been used for over a decade for a variety of material studies. Currently, ZR can produce a tailored current pulse to drive samples quasi-isentropically to pressures as high as 5 megabars. The purpose of this project was develop computational techniques, predictive capability, and high-fidelity point designs for Thor, Neptune, and other next-generation current-adder pulsed power accelerators.

We developed an optimization process for producing tailored current pulses, a requirement for many material studies, on the Thor generator. This technique, which is unique to the novel current-adder architecture that will be used by Thor, entirely avoids the iterative use of complex circuit models to converge to the desired electrical pulse. We used this procedure for the Thor design and developed a design for various materials of interest. Also, we extended these concepts to the megajoule-class Neptune machine design. Given this design, we were able to design shockless ramp-driven experiments of metals in the 10 Mbar range of pressure, higher than any previously reported experiments.

The computational results will aid in the design of powerful next-generation pulsed power accelerators that will play a key role in several DOE/NNSA missions, including science based stockpile stewardship.



## Predictive Modeling of Aging and Degradation of Materials in Extreme Environments

181060 | Year 2 of 2 | Principal Investigator: R. P. Dingreville

### Project Purpose:

The overall purpose of this project is to develop multiscale models that can simulate defect accumulation and subsequent macroscopic material property changes across a broad range of time and length scales. These models are then used to study radiation effects in a variety of metallic systems and radiation conditions, including neutron, light ion, and self-ion irradiation of nanolaminates, thin films, nano-grained materials, and bulk materials.

In order to accurately describe defect accumulation in nonhomogeneous microstructures and under complex irradiation conditions, simulation methods are needed that can explicitly account for the effect of nonhomogeneous microstructures on damage accumulation. In this project, an advanced simulation tool called spatially resolved stochastic cluster dynamics (SRSCD) has been developed for this purpose. This method is carried out by solving spatially resolved coupled rate equations of traditional rate theory methods in a kinetic Monte Carlo scheme. To enable the study of increasingly complex microstructures and irradiation conditions, several improvements were made to this method, including a pseudo-adaptive meshing scheme for cascade implantation and implementation of this method in a synchronous parallel kinetic Monte Carlo algorithm to allow large-scale simulations of radiation damage in polycrystalline materials. SRSCD was shown to be a good candidate for inclusion in a multiscale modeling hierarchy due to its increased computational efficiency compared to other methods such as object kinetic Monte Carlo (OKMC) while simulating more complex defect behaviors than most rate theory models.

## Time-Resolved X-Ray Diffraction Measurements on Laser-Compressed Polycrystalline Samples Using a Multi-Pulse, Short-Pulse Laser Generated X-Ray Source

191235 | Year 1 of 3 | Principal Investigator: M. Schollmeier

### Project Purpose:

In dynamic compression, materials may be compressed to stresses above phase transition pressures known from static studies, on time scales of nanoseconds to microseconds. For most materials, there are very few constraints on existing models for the kinetics or time-dependent nature of phase transitions under dynamic loading. We plan to investigate whether dynamic phase transitions are different from static ones and if material properties are affected by the kinetics of nanosecond to microsecond-scale compressions. Exploring the material structural dynamics can be performed with x-ray diffraction. We propose to perform time-resolved, x-ray diffraction measurements on dynamically compressed, polycrystalline matter. We will develop a multipulse, short-pulse laser-generated, high-energy ( $>10$  keV) x-ray source that would allow sub-nanosecond time resolution in dynamic x-ray diffraction (DXRD) experiments, which would be compatible with future experiments on the Z-machine. Material samples will be compressed using a separate, ns-duration laser pulse. We will use phase transitions in group IV elements or lanthanides, which occur at  $2\text{--}10$  GPa at room temperature, as examples to demonstrate time-resolved, multi-frame DXRD. These phase transitions are well characterized under static compression, but their crystal structure has never been directly observed under dynamic compression using nanosecond compression. DXRD will unambiguously demonstrate whether the phase transition occurs on dynamic (ns) timescales, determine the phase fractions of as a function of stress, and evaluate the precision of DXRD as a density diagnostic. DXRD will constrain multiphase equation-of-state models and set the stage for examinations of more complex phenomena such as material strength and kinetics.



## Wavelength Conversion Arrays for Optical and X-Ray Diagnostics at Z

173189 | Year 3 of 3 | Principal Investigator: E. J. Skogen

### Project Purpose:

Optical diagnostics play a central role in dynamic compression research, needed for equation of state development and phase transition studies crucial to our stockpile mission. Currently, streak cameras are employed to record temporal and spectroscopic information in single-event experiments. Optical signals streaked by the camera create a 2D record of the event, obtaining high temporal and spatial (spectrographic) resolution over relatively short time scales (0.1-10  $\mu$ s). These measurements are not easily achieved; however, equipment costs limit the experimental versatility, and limited readout elements constrain the tradeoff between temporal resolution and time duration. Furthermore, these cameras are at risk of becoming unsupported.

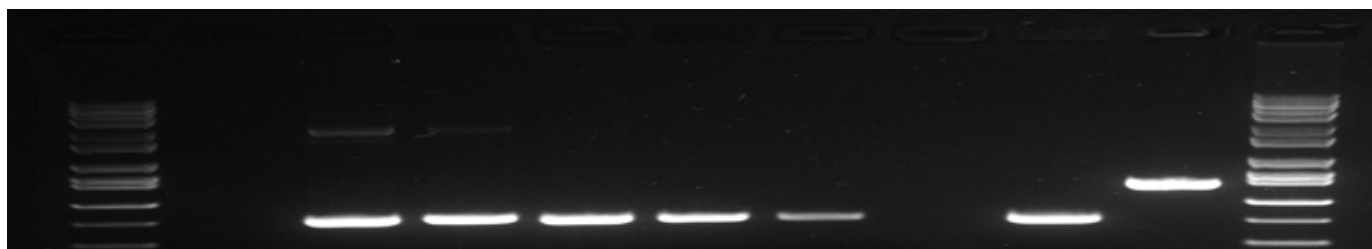
This project will solve the limitations that streak cameras impose on dynamic compression experiments while reducing both cost and risk (equipment and labor) by utilizing standard high-speed digitizers and commercial telecommunications equipment. The missing capability is conversion of experimental (visible/x-ray) wavelengths to the infrared wavelengths used in telecommunications. Although infrared-to-infrared wavelength converters exist, the concept has not applied to visible-to-infrared conversion technology.

We created an optical conversion array system that will allow new, more in-depth measurements than are currently being used. We leveraged the expertise of Sandia's photonic integrated circuit technology to develop a linear array of visible-to-infrared wavelength conversion circuits. The visible-to-infrared wavelength converter relies on Sandia's unique state-of-the-art photonic integrated circuit fabrication platform, which enables monolithic integration of more than 10 unique optoelectronic components on a single chip. Each optical wavelength converter in the array exploits this technology and is comprised of two optoelectronic active components: the photodiode (PD) and electroabsorption modulator (EAM). The PD is a light-to-current transducer; while the EAM is a voltage dependent transmission switch (higher reverse voltage leads to lower light transmission). Between the PD and the EAM resides a two-stage electrical amplifier which is used to amplify the signal received by the PD to a level useful to drive the EAM. We met the goals and completed a wavelength converter array system.





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## New Ideas

The New Ideas Investment Area aims to position Sandia to anticipate and respond to national security challenges (both now and in the future) by supporting high risk new ideas that have the potential to be transformational; for example, those with long time horizons, potentially high but as yet uncertain mission impacts, or nascent research in a new field that may in the future become transformational for our mission. It is intended to support leading-edge research that is outside Sandia's current research focus areas, but that may lead to breakthroughs in science and technology that could profoundly impact our national security mission.

*The image above is gel electrophoresis showing recovery of a DNA Test Message (TM) from various surfaces. The TM was spotted on the different surfaces, and swabbed the following day (~20 hours later). The swabs were assayed by polymerase chain reaction (a technique to generate many copies) and demonstrated the ability to recover the TM from the different surfaces. The results could lead to a potentially disruptive technology for securely storing and transferring sensitive, national security information. (Project 173140, Synthetic DNA for Highly Secure Information Storage and Transmission)*

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## A New All-Dielectric Nanolaser

191223 | Year 1 of 3 | Principal Investigator: M. B. Sinclair

### Project Purpose:

Countless applications in imaging, sensing, and communications would benefit from the availability of nanoscale, low-threshold, and high-confinement lasers. Traditional semiconductor lasers require complex epitaxy and are typically of microscale dimensions. While plasmonic nanolasers have recently been demonstrated, they are inherently hampered by metallic losses which preclude high-performance operation. We will explore an entirely new class of devices based upon subwavelength active dielectric resonators (DRs), potentially unlocking the promised benefits of nanolasers and related phenomena. Dielectric resonators have been intensively studied at Sandia and elsewhere, but remain passive devices. The development of active laser sources from traditional DRs is hampered by the low quality factor (Q) of their spectral resonances and by difficulties in fabricating resonators from appropriate active materials such as GaAs. Recent developments at Sandia provide a path for improving DR performance by: 1) greatly increasing the resonator quality factor (Q), and thereby greatly narrowing the spectral bandwidth; and 2) fabricating DRs from active materials such as GaAs/InGaAs. This project will capitalize on these two breakthroughs to develop tunable, narrow-band nanolasers with no metals in the cavity. Specifically, we will design high-Q DRs that contain embedded InGaAs gain layers and demonstrate optically pumped lasing. If successful, this work will provide the first ever demonstration of active DRs at optical frequencies and will serve as a first step towards the development of a new class of active DR based nanodevices including lasers; narrow band light sources; tunable, narrow band photon detectors; and sensors.

## Controlling Nanoparticle Assembly to Engineer New Materials

180922 | Year 2 of 3 | Principal Investigator: G. S. Grest

### Project Purpose:

Driving computer design integration of nanomaterials will enable transformation from a lab to fabrication within reasonable time and resources. We are developing a much needed means to significantly expedite computational pathways to design of nanomaterials while accounting for chemical information that is critical to their controlled integration. Currently, the assembly of nanoparticles is done through a time expensive random search of a large number of parameters including the nature of the nanoparticle itself coupled with surface encoding to drive integrations. Computer based material design has been proven to provide an effective tool to correlate a large number of parameters where in nanomanufacturing, particle size and shape, and different surface encodings are among the many variables which control direct nanoassembly.

A new effective computational method to define and access the relevant parameter space required to direct nanoparticles into well-defined arrays is being developed, establishing hierarchical coarse graining (HCG) pathways that reduce the number of objects required for computations, while retaining the essential interactions that control assembly. This innovative concept, defining how far coarse graining can propagate while retaining essential chemical information will be investigated. HCG will be able to probe mesoscopic length scales with chemical resolution while allowing an effective computational time to guide the design of nanoparticle assembly. This research will resolve a major barrier to computer design of nanoparticle integration, controlled dispersion and organizing of nanoparticles, while retaining their unique properties. This new approach will decrease computational time leading to effective screening that will significantly enhance nanomanufacturing.



## Creating and Understanding Lifelike Matter: Far-from-Equilibrium States that Arise from Injecting Energy into Dipolar Fluids

191215 | Year 1 of 1 | Principal Investigator: J. E. Martin

### Project Purpose:

The next frontier in physics is developing ways to create *functional* far-from-equilibrium states that are sustained by the continuous injection and dissipation of energy. Such driven dissipative systems can give rise to complex self-organization, such as occurs in the Belousov-Zhabotinsky reaction, in natural convection, and in living organisms. In fact, the fifth and last DOE Grand Challenge reads “*How do we characterize and control matter away—especially very far away—from equilibrium?*” The subtext continues, “*Discover the general principles describing and controlling systems far from equilibrium, enabling efficient and robust biologically inspired molecular machines...*”. To address this challenge, we plan to drive magnetic field energy into field-responsive fluids in such ways as to create vigorous noncontact fluid flows. Developing this capability will provide solutions to many problems, including noncontact heat and mass transfer in microgravity environments, microchannel mixing, active wetting, containerless massively parallel bioassays, fluid emulsification, and de-emulsification, dispersal of beneficial agents into liquids, and the extraction of contaminants from waste streams. This challenge has not yet been met because of the lack of a viable approach, but we have recently discovered that multi-axial, time-dependent magnetic fields can create vigorous, controlled fluid flow. Our experimental and theoretical project will lead to a predictive capability of how the field and fluid parameters can be exploited to create flows that address all of the issues raised above.

## Emergent Phenomena in Oxide Nanostructures

180923 | Year 2 of 3 | Principal Investigator: W. Pan

### Project Purpose:

The field of oxide electronics has seen tremendous growth over the past two decades and oxide materials have found wide-ranging applications in information storage, fuel cells, batteries, quantum sensing, and more, with potential for broader impact. In transition metal oxides, the strongly correlated d-electrons and interactions of spin, charge, orbit, and lattice degrees of freedom determine their physical properties. One of the most important phenomena in highly correlated oxides is the metal-insulator transition (MIT). Many novel devices utilizing MIT have been proposed, ranging from ultrafast switches for logic applications to energy dissipaters, thermal computation, quantum actuation, and more. Yet, despite this promise and many years of research, a complete understanding of the MIT remains elusive. Recently, we observed a novel electrical current induced MIT in self-assembled, vertically aligned epitaxial  $(\text{ZnO})_{0.5}:(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_{0.5}$  nanocomposite films. This current-induced MIT is totally unexpected and differs significantly from that observed in monophasic oxide films. In this project, we will conduct a systematic study of this MIT and aim to gain a solid understanding of the physics that underpins this transition. Moreover, emergent quantum phenomena due to the strong correlations and interactions among the charge, orbital, and spin degrees of freedom inherent in transition metal oxides will be explored.

We will study how oxygen annealing affects the observed MIT. In detail, we first study the transport properties in an as-grown sample at low temperatures and high magnetic fields. Then, we will anneal this same in an oxygen environment, and perform the same transport measurements. Aberration-corrected scanning electron microscope measurements will be carried out to correlate the structural and composition information with the transport results.

This work is nascent and exploratory. This research project requires expertise in the preparation of high-quality epitaxial oxide heterostructures, quantum transport measurements, and state-of-the-art aberration-corrected scanning transmission electron microscopy characterization, rarely found together in a single place.



## Mediated Flow Batteries

191225 | Year 1 of 2 | Principal Investigator: T. M. Anderson

### Project Purpose:

We aim to develop a mediated, lithium-based chemistry for flow batteries with higher energy density and improved performance and safety for stationary energy storage. The drive towards higher energy density, longer life, and lower cost batteries has exposed limitations in current technologies. This includes capacity of charge-storage materials that do not meet the cost and performance targets for utility markets as well as the need for increased renewables integration. Commercial insertion electrode materials do not meet these requirements because of the inherently limited amount of lithium that can be introduced into their stoichiometry. Likewise, conversion materials suffer from high resistances leading to large voltage losses. We plan to develop multivalent polyoxometalates (POMs) as lithium-storage materials and associated organic (or organometallic) redox shuttles for fast electron transfer. POMs differ from intercalation compounds in that they have higher operating voltages, and they are not subject to degradation over continuous cycling because lithium electrostatically attaches to their surface without major volume changes rather than full insertion into the bulk material. The mediators allow the POM to remain in the solid state during charging and discharging yielding higher energy densities and increased stabilities. The most significant technical challenges to implementing this concept are the voltage compatibility and electron transfer kinetics between the POM and the mediator, which we contend can be resolved by the highly tunable nature of both materials. If successful, this project is expected to yield more than an order of magnitude improvement in energy density.

Fundamentally new energy storage materials are crucial to meet the needs for providing power on demand. This project pushes the limits of current flow battery technologies. Our research addresses the challenge of changing the mindset of what can conceivably make a better battery.

## Probing Small-Molecule Degradation to Counter Enzyme Promiscuity

173142 | Year 3 of 3 | Principal Investigator: S. Rempe

### Project Purpose:

Enzymes that degrade specific small molecules could save lives by neutralizing threats from chemical agents in the blood or environment, but promiscuous interactions with other molecules typically limit their effectiveness by blocking the enzyme active site. An obvious solution is to re-engineer the enzyme to enhance catalytic fidelity, but lack of understanding about how enzymes discriminate between molecules remains a formidable challenge to this approach. Our recent work in collaboration with University of Texas (UT) suggests a new approach and a model system for understanding enzyme specificity. Asparaginase enzymes catalyze degradation of asparagine, which forms the basis of a medical treatment. Competition by other abundant molecules interferes with asparagine decomposition, thus hindering enzyme efficacy. Asparaginase is advantageous as a model degradation enzyme because variants that demonstrate different binding affinities and catalytic rates can be compared. Our preliminary work suggests that the mechanism of molecular specificity in asparaginase depends on a different set of chemical interactions than previously speculated. We have leveraged Sandia's strengths in molecular simulation and UT experimental expertise in asparaginase modification and functional assays to understand enzyme degradation of small molecules. Our simulations probe how local properties of the asparaginase active site determine molecular binding affinities and free energy barriers to degradation, and predict mutations (tested experimentally) to tune catalysis to favor a specific molecule.

The project led to the development of a new strategy to re-engineer safer and more effective enzymes to break down small molecules. That strategy was demonstrated for a leukemia drug, with potential therapeutic applications to leukemia and other cancer cells. The strategy is broadly applicable to improve enzymes that break down chemical warfare agents for therapeutic and decontamination applications.





## Sandia's RVCC Technology: A Pathway to Ultrahigh Efficiency Building Air Conditioning, Heating, and Refrigeration

180924 | Year 2 of 3 | Principal Investigator: H. A. Kariya

### Project Purpose:

A large fraction of US energy consumption is due to space heating and cooling in the residential and commercial sectors. Currently, vapor compression cycles (VCCs) are used widely for heating and cooling due to their robustness and ability to heat or cool greater than the energy supplied (coefficient of performance  $>1$ ). However, real world VCCs deviate substantially from the Carnot efficiency due to loss mechanisms such as parasitic thermal resistance, excessive vapor superheating, and chaotic refrigerant two-phase flow behavior. Prominent thermal parasitics in VCCs include the thermal resistance between the heat exchanger fins and ambient air and the added thermal resistance associated with evaporator frost formation. Furthermore, the widespread use of vapor superheating to prevent liquid from entering the compressor generates additional entropy. Undesirable phase-change flow patterns in high aspect ratio channels prevent effective vapor (liquid) escape in evaporators (condensers), impairing heat transfer and increasing pressure drop in the flow. The rotary vapor compression cycle (RVCC) embodies a radical rethinking of conventional VCCs, wherein the condenser, throttle valve, evaporator, and compressor rotate at high speed on a common axis to counteract the above sources of inefficiencies. Rotation of the evaporator and condenser results in enhanced airside heat transfer. Rotation of the refrigerant is expected to separate the liquid and vapor phases through centrifugal and Coriolis forces, and this separation is predicted to improve heat transfer in the refrigerant flow and prevent liquid from entering the compressor. Through this project, we will experimentally study the uninvestigated regime of two-phase flow in the rotating frame. The evaporating and condensing flows will first be characterized through video imaging and subsequently the heat transfer in the flows will be analyzed with infrared thermography. The new understanding will make it possible to explore and optimize proof-of-concept designs for RVCC.

## Synthetic DNA for Highly Secure Information Storage and Transmission

173140 | Year 3 of 3 | Principal Investigator: G. Bachand

### Project Purpose:

Protection of information is one of the greatest challenges to our Nation's security, and will continue to be for the foreseeable future. In particular, digital storage and transmission has proven increasingly susceptible to compromise, necessitating the development of disruptive technologies to secure highly sensitive information. The use of synthesized DNA to store digital information with high capacity and low maintenance was recently reported, representing a novel paradigm for information storage, particularly as DNA can be stably stored for tens of thousands years. This system, however, also offers the ability to transmit information in a highly secure biomolecule, as opposed to an encrypted digital format. The work on this project was driven by the question—can synthetic DNA be used as a game-changing approach to transmit and store sensitive information? Our approach specifically borrowed from nature's means of translating genomic information into functional units to encrypt data in a highly secure manner. The ability to encode digital data in synthetic DNA has been based on conversion of binary data into DNA base pairs. In our work, we developed a means by which alphanumeric text could be directly translated into DNA language. The security underlying our approach involves the potential generation of up to an infinite number of unique translations keys (i.e., 256-factorial for quadruplet codons) for each message. Our approach also addressed critical issues with respect to character/word frequency and reducing repeated DNA sequences (which make the DNA difficult to synthesize and sequence). This project aligns with enhancing Sandia's ability to address future national security needs by developing a potentially disruptive technology for the safe and secure storage of national security information using synthetic DNA. Work on this project will provide the foundational R&D necessary to demonstrate the proof-of-principle for the national security community.



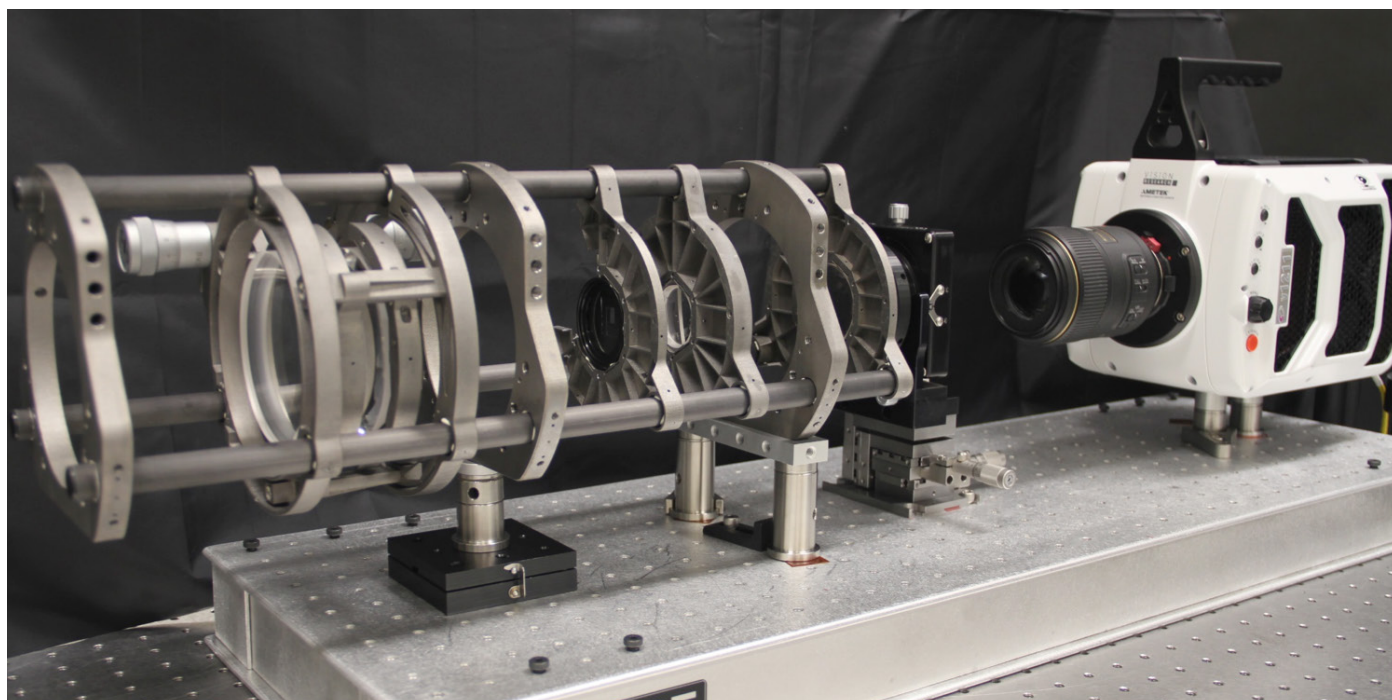
## Topological Photonics: The Quest for Ultimate Photon Control

191221 | Year 1 of 3 | Principal Investigator: G. S. Subramania

### Project Purpose:

Topological insulators are systems where electrons conduct only at the edges and surfaces due to edge states within the bandgap. These states are topologically protected and propagate scatter free, making them interesting for robust quantum computing. Recently there has been great interest in their electromagnetic analog namely topological photonic structures (TPS). They can possess topologically protected photonic modes that can propagate unidirectionally without scattering and can have an extreme photonic density of states (PDOS). These unique properties can directly impact many photonic systems used in quantum information processing applications such as single photon transport. Several theoretical works and experimental demonstrations of topological states have been done on macroscopic systems such as optical fiber arrays and microwave structures. Some recent progress has been made on chip-scale demonstrations but mostly for optical isolators. However, chip-scale demonstration of truly topological photonic structures showing scatter-free protected states would be highly game-changing for many photonic applications. Here we plan to demonstrate, in a chip scale 2D photonic crystal (PC) system, scatter-free edge states by dynamic modulation of arrays of coupled PC cavities. This area is very new with many fundamental questions related to the photonic quantum hall effect and the photonic quantum spin hall effect.

Topological photonics can enable ultimate photon control such as scatter-free propagation, nonreciprocity enabled by topological protection for quantum light control and information. This is an emerging area with mostly theoretical work and few experimental demonstrations. This project will leverage Sandia's established strength in nanophotonics to achieve fundamental understanding through experiments that ultimately position us strongly for future mission needs. Understanding the challenges of achieving photonic topological properties will impact the science and engineering of quantum computing.



## Defense Systems and Assessments

The Defense Systems and Assessments Investment Area (IA) delivers advanced science and technology solutions to deter, detect, track, defeat, and defend against threats to our national security. The work includes the development of innovative systems, sensors, and technologies for the nation's defense communities. This IA seeks to draw upon Sandia's state-of-the-art ST&E capabilities through focused investments in four strategic program areas: Synergistic Defense Products (SDP), National Security Space Innovations (NSSI), Cyber, and Global Nuclear Assurance Security (GNAS). SDP is focused on developing leading edge technologies and capabilities to respond to emergent national security challenges and is synergistic with NW mission. NSSI develops and exploits innovative space sensing systems to address critical National Security challenges. Cyber delivers science and engineering based cyber technologies to continuously advance national security missions. GNAS enables the US government to confidently anticipate, assess, and address nuclear risks worldwide through the use of advanced systems and technologies, expertise, and situational awareness systems/tools.

*The image above shows a plenoptic camera, which captures information about the light field radiating from a scene, developed for optical remote sensing of spectral-temporal signals. Improving the capability to design systems that observe and analyze the spectral signals of fast transient events benefit many national security missions. (Project 173056, Co-Design of Sensors and Analysis Methods for Optical Remote Sensing of Spectral-Temporal Signals)*

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## Accurate Characterization of Real Networks from Inaccurate Measurements

191009 | Year 1 of 2 | Principal Investigator: A. Pinar

### Project Purpose:

We propose to develop provably accurate algorithms that can characterize the structure of an information network despite limited and biased measurements. Our nation's dependence on information networks makes it vital to anticipate disruptions or find weaknesses in these networks. But networks like the Internet are vast, distributed, and there is no mechanism to completely collect their structure. We are restricted to specific data collection schemes (like traceroute samples from router interfaces) that examine tiny portions of such a network. It has been empirically documented and theoretically proven that these measurements have significant biases, and direct inferences from them will be wrong. But these data collection mechanisms have limited flexibility and cannot be easily modified. Moreover, in many applications there are limits on how much data can be collected.

How do we make provably accurate inferences of network properties with biased and limited measurements? To address this problem, we propose to use techniques from sublinear graph sampling, which is an emerging area in theoretical computer science. Our aim is to understand what graph properties can be provably and accurately determined by sampling a graph using available data collection mechanisms. Our methods provide a systematic, rigorous, and scientific approach to understand the structure of information networks. Current measurements are biased and we need to remove these biases by clever sampling. Our project will produce algorithms and tools that accurately represent system topology, and will give measurements of a network. This is important for protecting our information networks for national security.

## Adaptive Waveform and Signal Processing Techniques that Mitigate Adversarial Anti-Access/Area Denial (A2AD) Technology

173066 | Year 3 of 3 | Principal Investigator: C. Musgrove

### Project Purpose:

Recent research and development efforts and proliferation of electronic warfare (EW) technologies have strengthened Adversarial Anti-Access/Area Denial (A2/AD) capabilities. These threats pose a significant risk to our national security missions that rely on intelligence, surveillance and reconnaissance (ISR) systems. Advanced A2/AD technologies pose a substantial risk to ISR applications such as coherent radar imaging that use predictable waveforms like linear FM chirps. The objective of this project is to develop techniques that can defeat select adversarial A2/AD technologies and maintain mission performance (image quality and image production rate). This project will focus on developing waveforms and signal processing techniques for Electronic Counter-Countermeasures (ECCM). Challenges associated with defeating A2/AD systems include developing adaptive waveforms and signal processing techniques, interference rejection, false target discrimination, statistical signal and image processing, and reducing computational loads associated with adaptive signal processing.

## Advanced Detection and Focusing of "Peak Through" SAR Imagery in Foliage

180853 | Year 2 of 2 | Principal Investigator: D. L. Bickel

### Project Purpose:

This research investigated observation of objects concealed under foliage at higher radar frequencies, specifically X-band and above. Sandia has developed both low and high frequency imaging radar systems, with most of the radar systems being at higher frequencies. Because typical radar investigations are at much lower frequencies due to propagation attenuation, there is a need to understand what benefit, if any, there is in "peak through" of foliage at these higher frequencies?

This limited study collected real data with Sandia imaging testbed radar systems using both an X-band fully polarized and a Ka-band single polarization. We investigated detection of a vehicle concealed under available foliage (bosque cottonwoods and pecan orchards) using flight test radar data. A couple of new techniques using coherence and polarization differences between man-made and foliage were developed. Initial results look promising, but these techniques need to be examined with additional foliage types. In addition, some study of the distortion caused by the signal passing through the foliage was performed for the X-band multi-polarization system using receivers under the foliage and in the clearing. Also, a preliminary investigation into focusing of images distorted by propagation in foliage was performed.



## Alternate FPA Architectures

190995 | Year 1 of 2 | Principal Investigator: E. R. Olson

### Project Purpose:

The purpose of this project is to investigate new areas of development, both conceptual and theoretical, in the field of focal plane array (FPA) performance. Some of the questions that inspired this research are:

1. How can we improve the dynamic range and bit depth of image sensors?
2. How can we increase the sampling rate of image sensors?
3. How can we reduce the power consumption of image sensors?
4. Are there any new concepts that can be used to extend the mission space of an image sensor without complicating the design, and increasing the cost?

Addressing these questions with new approaches will potentially benefit national security areas that utilize image sensors, boosting capabilities and widening mission space.

The intent and scope of this project is to produce several new ideas that will be simulated, modeled, and even tested in the laboratory. The S&T question will be addressed through the results gained from the circuit modeling and laboratory testing. These results will be used in further modeling to propose new advanced uses for these high performance circuits. The feasibility of these circuits will be first demonstrated on a circuit board design which will be built and tested. Secondly, the feasibility of constructing these circuits in an actual FPA design will be demonstrated through an actual integrated circuit design, without the fabrication process.

This project is different from other FPA-based projects in that it has already proposed several new concepts for addressing a wide variety of performance metrics for image sensors. These ideas have stemmed from lessons learned from previous research, as well as major research efforts that exist today that are already pushing the technological limits.

## Alumina Materials Chemistry

180854 | Year 2 of 2 | Principal Investigator: D. Kammler

### Project Purpose:

Material property changes are accompanied by microstructural changes. Diamonite, a 94% alumina, is a structural ceramic with a pink color resulting from the presence of about 0.5% Cr, which might provide a valuable signal useful for inline process control. The goal of this project is to assess the potential of small process or chemistry changes to produce significant changes in properties without significantly altering microstructure. Small changes to the pink diamonite chemistry, including changes to trace constituent (Cr and Fe) concentrations, were evaluated.

After developing a process for fabricating an alumina similar to diamonite, modified and baseline test coupons were produced. Common characterization methods such as x-ray diffraction and scanning electron microscopy revealed that the control and modified coupons did not differ with respect to phases present, grain size distribution, or other easily observable microstructural features. Slight differences in the shade of pink color were quantified using diffuse reflectance measurements. Additional measurements at an x-ray Synchrotron facility revealed that a significant portion of these observed differences in diffuse reflectance correlated with changes to the concentration and/or oxidation state of the Fe present in both the baseline and modified diamonite. Subtle changes to the batch chemistry and process ambient changes could be used to change how Fe was partitioned between the 6% intergranular glassy phase in diamonite and small ~5-25um Fe-rich precipitates. Color (quantified via diffuse reflectance) was found to be tunable with minimal microstructural change.

The intergranular phase in 94% aluminas, like diamonite, enables densification at lower process temperature via liquid phase sintering and can flow around and bond to metallize, thereby enabling ceramic-to-metal brazing. Here, the intergranular phase has been modified to be sensitive to kiln ambient without significant microstructure change, thereby increasing its usefulness. Given that similar relationships likely exist in other aluminas, this result is probably broadly applicable. Low-cost built-in process monitoring schemes like this could improve the manufactured quality of a variety of alumina containing articles.



## Assessing the Security Impact of Moving Target Defense (MTD) Approaches

173071 | Year 3 of 3 | Principal Investigator: B. P. Van Leeuwen

### Project Purpose:

Moving target defense (MTD) approaches promise to increase complexity and cost for attackers by continually changing the operating cyber environments. However, MTD security impact to the overall networked system is largely unexamined. Dynamic reconfiguration of computing elements and their connectivity must take into consideration the stability and security impact to the overall networked system. While an attacker may encounter unpredictability in a MTD environment, system administrators must assure stability and overall security of the changing environment. Current MTD techniques assume that the effect of change is contained, localized, and does not have any adverse impact to system-wide operation and security.

The idea of MTD caught the attention of a large number of computer network security researchers, with numerous MTD techniques proposed in scientific research papers. A 2014 research paper noted an initial survey that identified greater than 120 academic papers describing various MTD techniques and approaches. Since then, research papers have proposed additional MTD approaches. However, to date, few MTD approaches have been implemented in operational systems. A partial reason for the limited deployment of MTD in operational systems is the lack of practical experience in deploying MTD and the lack of analytics describing the effectiveness of proposed MTD techniques and approaches.

One aspect of deploying MTD in a system is its cost of deployment or defensive work factor. Another aspect is the MTD's ability to enable security and thwart attacks. This research project developed a capability to assess the effectiveness and security impacts of MTD techniques in an operational-like environment. Techniques to evaluate the effectiveness of MTD approaches to secure a network were also identified and developed. The developed capability varied from other MTD analysis approaches in that it incorporated actual MTD deployments in operational-like modeled environments and measured both defensive costs and security benefits.

## Assessment of Nontraditional Phenomenologies for Proliferation Detection

190997 | Year 1 of 3 | Principal Investigator: T. J. Kulp

### Project Purpose:

This project is a research effort to identify and create fundamental understanding of nontraditional phenomenologies and sensing technologies to detect nuclear weapons proliferation. This work targets weapons-production activities that are not within the current sphere of interest of external organizations (such as NNSA), which typically focus on detecting weapons-material fabrication. A basic premise of this work is that new technologies and modalities exist for recognizing activities associated with nuclear proliferation, but that they have not been utilized because reliance on the National Technical Means infrastructure often drives advances in existing paradigms.

Examples of activities to be considered include operations associated with weaponization (material movement, hydrotesting, and generation of associated subsystems such as firing sets), graduation from fissile to thermonuclear device testing, detection of material mining, and development of delivery systems. These are of particular interest because they draw on Sandia's weapons program knowledge base. The effort will also draw guidance from the recent Defense Sciences Board report on Nuclear Proliferation Detection, which emphasized the exploration of nontraditional activities such as were applied to improvised explosive devices (IED) fabrication. The US IED response system will be analyzed to provide lessons learned and to stimulate the use of novel methods (big data, behavior analysis).



## Broadband Digital AESA Radar Prototype for Multi-Mission ISR Applications

173060 | Year 3 of 3 | Principal Investigator: H. Loui

### Project Purpose:

The purpose of the project was to develop a broadband active electronically scanned array (AESA) radar prototype for intelligence, surveillance, and reconnaissance (ISR) applications to counter anti-access/area denial strategies that may actively jam, spoof, or interfere with front-line electromagnetic sensors.

Multi-purpose, multi-mission, threat du jour radars with large instantaneous bandwidth are desired by many government agencies. These types of radar systems may offer low-latency, high-resolution data products for efficient target identification and tracking and can utilize arbitrary waveforms with adaptive beam formation to mitigate jamming and detection. Such levels of performance can only be achieved at low cost by way of an ultra wide-band (UWB) AESA that reduces radio frequency (RF) component count, utilizes commercial-off-the-shelf parts, and leverages existing research and development efforts. Unfortunately, the lack of practical, compact, low-loss, broadband, high-resolution radio frequency (RF) beam steering devices limits system performance and results in complex mission-specific radars that are costly to develop, maintain, and upgrade.

The S&T question that inspired us to do this research is: how to enable electronic beam steering of UWB sensors for improved ISR in denied environments? The intent and scope of the research throughout the duration of this project have been to demonstrate that lower cost, broadband, software-configurable, AESA-based mission-agile radars can be built without the use of RF analog phase shifters (APSSs) and true-time-delay (TTD) devices that limit bandwidth, reduce efficiency, and constrain electronic beam steering performance of existing electromagnetic sensors.

## Co-Design of Sensors and Analysis Methods for Optical Remote Sensing of Spectral-Temporal Signals

173056 | Year 3 of 3 | Principal Investigator: M. W. Smith

### Project Purpose:

We proposed to create and demonstrate a new process for co-designing remote sensing instruments and the accompanying data analysis methods for application to spectral-temporal signals. Events, or signal sources, are generally the items of primary interest when data is collected remotely by a sensor. The collection and analysis of signals are means to the end goal of retrieving information about the signal sources. We postulated that sensors and analysis methods should be designed together to produce a system that efficiently delivers high value information. We believed that field measurements and phenomenology models should be used to identify important features in the signals prior to designing a sensor. We worked with two classes of events that produce transient spectral-temporal optical signals—lightning and small chemical explosions—to develop and demonstrate the co-design process. Lightning is a ubiquitous background signal in optical remote sensing and there is wide application for determining munition characteristics from optical signatures. Our co-design approach stands in contrast to the practice of designing sensors based on simple signal-to-noise ratio (SNR) and related metrics. The end result of the prevailing practice can be a system that collects enormous volumes of data in multiple channels with high inter-channel correlation, expending more resources than necessary while perhaps still failing to capture key information. Our co-design process has led to the creation of a highly efficient new sensor. This sensor, a high speed, multichannel plenoptic camera, produces relatively compact data volumes that contain the key information required to draw conclusions about the events that produced the signals that were observed.



## Confidence in Cyber Modeling and Simulation

180830 | Year 2 of 3 | Principal Investigator: S. T. Jones

### Project Purpose:

Understanding the range of behaviors that cyber systems exhibit in response to their inputs and environment, especially those that are rare or malicious, is critical for many national security applications. Sandia-developed, emulation-based cyber models are actively being utilized by multiple agencies to inform their decisions. Unfortunately, we don't know how well these models capture the behavior of the real world systems they represent. Using unvalidated models for decision making is fraught with risk.

Verification and validation (V&V) techniques address exactly this problem by systematically building a credibility case for a model based on evidence derived from comparisons between model predictions and experimental outcomes. Well-accepted V&V processes have been developed for other model-rich application domains like nuclear weapons and aerospace. No V&V process for emulation-based cyber models exists.

Ideally, we would base a V&V process for cyber models on existing practice. That is our approach for this project. So far, we have found that general V&V techniques are a good fit for emulation-based cyber models with a few notable exceptions. Our research has focused on finding these gaps and bridging them with new techniques suitable for the cyber domain.

The endeavor is high risk. Most interesting cyber scenarios may be "unvalidatable" (see Hodges and Dewar 1992). Additionally, V&V may lead us to invalidate past models. Complete success comes through the creation of an effective and economical V&V process, which will build appropriate credibility and mitigate risk for both Sandia-developed and others' models. As in other domains where measurement and evaluation techniques are introduced for the first time, we expect that adoption of cyber modeling V&V metrics and feedback will enable rapid advances in the development and practice of cybersecurity modeling and simulation.

## DISeG: Data Inferencing on Semantic Graphs

180834 | Year 2 of 2 | Principal Investigator: J. D. Wendt

### Project Purpose:

Standard node/edge graphs are often insufficient for representing complex real-world data. Semantic graphs can be used to more accurately represent reality by adding attributes and relationship types to nodes and edges. However, solving complex equations (e.g., global function minimization) on such graphs and subsequently understanding the effect of various elements in the graph are open research. To solve such problems, two general solution techniques are typically employed: 1) either ignore the semantic information and solve using standard graph techniques or 2) solve using a standard graph technique for each semantic "layer" (for all nodes and edges of a specific type) and merge the results. Both solutions are incomplete as the first ignores all semantic information stored in the graph and the latter ignores cross-type information flows.

We propose that existing data inferencing techniques (e.g., belief propagation, Bayesian networks, etc.) be mapped to semantic graph problems. Furthermore, we will analyze the inferencing results using information-theoretic metrics to understand how influential nodes and subgraphs affect the rest of the graph. These techniques can be used in multiple application domains including supply-chain risk management (SCRM). In SCRM, with only a few "good" and "bad" companies and key personnel, unlabeled suppliers can be ranked based on semantic relationships to the labeled nodes. Other critical national security problems benefitted by inferencing on semantic graphs include—but are not limited to—computer network analysis and social media analytics.





## Deployable, Ground-Based, Discrete Zoom Telescope

173059 | Year 3 of 3 | Principal Investigator: E. G. Winrow

### Project Purpose:

The development environment for optical systems, either ground, air-, or space-borne, is constantly seeking lighter, cheaper, and more quickly developed systems without sacrificing mission performance. Here, a development methodology for a telescope system is presented to address those needs. A single detector system with a 10x zoom was baselined to address typical missions requiring both large area scanning and detailed target characterization. Novel approaches to development include extensive use of 3D printed components, modular structure design, simple-shape design of carbon fiber structures, precision active alignment of optics in imprecise structures, precision lens positioning with crude motion systems, topological optimization of structures, and image correction algorithms to enhance moderately precise optics.

This project has inspired design methodologies used in the Plenoptic Camera LDRD project (Smith), GPS Prime SIGHTS optical design and alignment plans, and several proposals for future satellite optical systems. This project also developed a new capability in the Horizontal Alignment Tool (HAT) for active alignment of optical systems in a native horizontal position. New capabilities for design of structures using 3D printed hardware and COTS carbon fiber structural elements were also developed. Additionally, a new method for low cost, high precision optical alignment was developed and is being implemented in several current programs, and anticipated to benefit future programs.

## Dim Target Tracking using an Adaptively Tuned Velocity Matched Filter on High Performance Computing using A Priori Information for Real-Time Tracking

180839 | Year 2 of 2 | Principal Investigator: D. K. Melgaard

### Project Purpose:

The purpose of this project was to extend our detection capabilities for real-time detection of moving target signatures for staring sensors, which is a critical gap in many space and remote sensing missions. A specific area needing attention was for targets that present themselves as streaks rather than points. For staring sensors, these target signatures are the result of an integration time that is long, relative to the velocity of the target. Consequently, our research first focused on finding algorithms to enhance the signal-to-noise ratio (SNR) of the streaks. We created, improved, and evaluated several types of algorithms including track before detect approaches for that purpose. These algorithms included velocity-matched filters (VMF), steerable filters, phase congruency and a new dynamic programming algorithm, recursive estimation of velocities, energies, and locations intra-frame projection (REVEAL-IFP). VMF demonstrated significant improvements in improving the SNR, but exhaustive searches of the hypothesis space can be intractable. The steerable filters employ specialized basis filters to reduce the computational load for determining orientation. Phase congruency uses wavelets to find and display the common phase inherent in moving targets to reveal the location and direction of the target. REVEAL-IFP (developed at Sandia) fuses repeated motion models to improve the detection. These algorithms all improved the SNR of the streak, but depending on the type of background, also produced artifacts that affected the detection of the streaks. The next phase in our research was to investigate algorithms to detect the streaks and characterize their performance. The Hough and Radon transforms are well known for locating lines in images, so we analyzed their effectiveness. In the process of that investigation, an alternative method we refer to as contiguous region-based detection was developed. Finally, we evaluated the algorithms for real-time environments. Our analysis indicated that real-time execution could be achieved using high performance computing and parallelization.



## Dynamic Analytical Capability to Better Understand and Anticipate Extremist Shifts within Populations under Authoritarian Regimes

173067 | Year 3 of 3 | Principal Investigator: M. L. Bernard

### Project Purpose:

The US' inability to adequately assess geopolitical and sociocultural dynamics of extremist groups has led to failures in understanding, anticipating, and effectively responding to shifts in their movements and allegiances. Recent attacks within the US highlight the need to more precisely understand and anticipate changes in societal attitudes and behaviors due to radicalization. This is particularly important as new al-Qaeda cells and affiliates have sprung up in Southeast Asia and Somalia. A significant concern is their stated intent and effort to plan and conduct terrorist attacks against the US.

We proposed to develop a generalizable data- and theory-supported capability to better understand and anticipate (with quantifiable uncertainty): 1) how the dynamics of allegiance formations between various groups and society are impacted by active conflict and by third-party interventions and 2) how/why extremist allegiances co-evolve over time due to changing geopolitical, sociocultural, and military conditions.

Working with analysts, we developed a standalone computational assessment tool for evaluating dynamic military, geopolitical, and socioeconomic interaction effects of extremist groups. Using engineering and social science validation techniques, this effort will produce a capability to quantifiably assess current events and choice options ("what-if" queries) concerning geopolitical inter-group/regional dynamics within a distribution of likely rest-of-the-world reactions to investigate underlying attitudinal and behavioral (extremist) shifts across time. The resulting structure was designed to be broadly applicable across different ethnic, political, and social groups and will focus on specific extremist group behaviors in response to military, social, economic, and political intercessions.

This effort provided a fundamental R&D capability that greatly expands current state-of-the-art tools. To have a true capability that can fully assess group interaction effects with quantifiable uncertainty, this effort developed a world-class analytical system that assesses multiple scales of extremist group behavior (from military/political organizations to societal interactions) associated with the external (geopolitical, physical, and socioeconomic) world.

## Dynamic Multi-Sensor Multi-Mission Optimal Planning Tool

180833 | Year 2 of 2 | Principal Investigator: C. G. Valicka

### Project Purpose:

Remote sensing systems have firmly established a role in providing immense value to commercial industry, scientific exploration, and national security. Continued maturation of sensing technology has reduced the cost of deploying highly capable sensors while at the same time increased reliance on the information these sensors can provide. The demand for time on these sensors is unlikely to diminish. Coordination of next-generation sensor systems, larger constellations of satellites, unmanned aerial vehicles, ground telescopes, etc., is prohibitively complex for existing heuristics-based scheduling techniques. In collaboration with Texas A&M University, we have developed algorithms and software for collection scheduling, remote sensor field-of-view pointing models, and bandwidth-constrained prioritization of sensor data. Our approach followed best practices from the operations research and computational geometry communities. These models provide several advantages over state-of-the-art techniques. In particular, our approach is more flexible compared to heuristics that tightly couple models and solution techniques. First, our mixed-integer linear models afford a rigorous analysis so that sensor planners can quantitatively describe a schedule relative to the best possible. Optimal or near-optimal schedules can be produced with commercial solvers in operational run-times. These models can be modified and extended to incorporate different scheduling and resource constraints and objective function definitions. Further, we have extended these models to proactively schedule sensors under weather and ad hoc collection uncertainty. This approach stands in contrast to existing deterministic schedulers which assume a single future weather or ad hoc collection scenario. The field-of-view pointing algorithm produces a mosaic with the fewest number of images required to fully cover a region of interest. The bandwidth-constrained algorithms find the highest priority information that can be transmitted. Experiments conducted using the developed models, commercial solvers, and benchmark datasets have demonstrated that proactively scheduling against uncertainty regularly and significantly outperforms deterministic schedulers.



## Efficient-Track-Before-Detect with Minimal Prior Knowledge

195968 | Year 1 of 2 | Principal Investigator: K. Merry

### Project Purpose:

The last decade has seen a tremendous proliferation of sensors designed to provide wide area surveillance using a range of spectral bands and frame rates to address a variety of mission challenges. These sensors produce massive volumes of exploitable data. Our research is focused on determining whether the data from this class of sensors can be processed using highly efficient dynamic programming techniques, specifically with the goal of enabling real-time processing with modest hardware.

The fundamental problem is one of associating several low-confidence signatures to identify combinations that have a high likelihood of being a signature of interest. Existing state-of-the-art techniques attempt to solve this problem by brute force search constrained by an expected target motion model. This family of algorithms has struggled to scale to the large data rates of modern sensors.

In contrast, the dynamic programming-based approach is capable of efficiently scanning large streams of data to identify patterns of interest. It shows promise in the ability to associate sets of low-confidence returns over longer timescales and with more flexible motion models than the brute force methods.

In our first half-year, we evaluated the performance of our dynamic programming-based approach against the traditional methods on a variety of datasets from two sensor platforms—one operational and one simulated. We found that the dynamic programming approach exceeds the detection performance of all uncued detection algorithms that we tested, as well as the cued algorithms which are feasible to run in real time. In FY 2017, we plan to gather datasets from additional sensor platforms. However, the primary goal will be to develop and assess additional sensor- and target-agnostic modifications that can be used to further improve detection performance while maintaining the real time computational capability.

## Engineering Efficient Human-System Interaction in Defense Systems-of-Systems

180856 | Year 2 of 3 | Principal Investigator: M. J. Hoffman

### Project Purpose:

We are developing a capability for quantification of human-technology interactions within system-of-systems engineering. Engineering complex systems-of-systems typically does not include initial consideration of how humans will interact with the system-of-systems' heterogeneous constituent technologies/systems. But these interactions have vital effects on overall system-of-systems functionality; quantitative understanding of these effects and their propagation through the system over time can provide significant cost and performance improvements, and possibly save lives.

In general, human-technology interactions are handled through training, after design engineering is complete and systems are fielded. *Prior* to system fielding, understanding where technology might benefit human performance in a system-of-systems (e.g., where automation and task augmentation is beneficial) is very limited. Similarly, ranges of potential operators' knowledge, skills, and abilities are not always adequately considered in understanding system performance at the design stage. When assessing effectiveness metrics like troop-to-task ratio (critical in military system-of-systems engineering), quantifying such effects is essential.

Sandia has significant capability in quantitative system-of-systems modeling; this capability enables understanding technology/system and system-of-systems effectiveness when engineering complex system-of-systems. However, this capability has not included (with adequate fidelity) human entities, which are necessary to understand effects of human-technology interaction within the system-of-systems context. We are working to expand Sandia's existing system-of-systems modeling capabilities to include this fidelity, by incorporating Sandia's expertise in quantifying/modeling human behavior and behavioral effects on interactions with technology. We are using the engineering of a representative military forward operating base (FOB) as the system-of-systems use case for researching the quantification of human-technology interaction effectiveness.

Quantifying the impacts of technology on human performance (and vice-versa) as part of evaluating system-of-systems effectiveness is a novel area of research with very few existing capabilities but many important applications. Developing and demonstrating credible fundamental/prototype capability in this area will distinguish Sandia and allow Sandia to pursue new partnerships where human-technology issues are fundamental, both in DOE and DoD.



## Event Correlation using Spatio-Temporal Point Processes

196390 | Year 1 of 3 | Principal Investigator: J. D. Tucker

### Project Purpose:

In many critical intelligence and surveillance applications, a high degree of operator intervention is currently required for all-source analysts attempting to interpret events and findings through space and time. Metadata overlays must be assembled manually, and complex database queries must be constructed. Thorough exploitation remains elusive due to the ever-increasing volume of processed sensor data. To more efficiently capture correlations in large volumes of detected event data, we propose to apply modern spatiotemporal point process models and advanced statistical inference. Our approach will bring mathematical rigor to this subset of “data mining” problems and improve sensor exploitation across a range of missions.

Recent studies in epidemiology have used spatial point processes to model the spread of disease across regions of interest, and several papers have incorporated spatiotemporal aspects in the model development and parameter estimation stages. While such hybrid approaches have been successfully applied to a variety of disease cases, we could not find evidence of successful extension to mission relevant sensing problems. Furthermore, very little effort has been applied to looking at correlations between events across both space and time—and making inferences from these relationships.

Our hypothesis is that extending spatiotemporal point process methodologies to develop inferences about the correlation of events in both space and time will provide a more complete and nuanced picture to the analyst in near-real time. We propose to develop models from spatial point process theory, with corresponding estimators to make inferences and communicate the patterns in a manner that is concise and informative.

The proposed research involves the exploration of a new method of correlating events in both space and time. We will use a nonparametric approach in developing a self-exciting intensity model and the estimation of the parameters will take missing data into account.

## Exploitation of Optical Polarimetry for Remote Sensing

180840 | Year 2 of 3 | Principal Investigator: J. M. Craven

### Project Purpose:

Investments have been made by multiple government agencies to produce optical remote sensing systems with polarimetric measurement architectures. However, due to limited effort and rigor in characterization and validation, a comprehensive understanding of the capabilities of many of these systems is lacking. Furthermore, the utility of polarization data products for remote sensing missions remains relatively unclear. A frequently cited application is improved contrast for detection of inherently polarized manmade objects against weakly polarized natural scenes. However, the effectiveness of even this regularly cited example has not been well-quantified, and the general utility of a given polarimeter in situations that an operational system will encounter such as low light, long standoff distances, bad weather, etc., remains unknown. Furthermore, whether polarization signatures can provide some exceptional utility that more established sensing modalities cannot cover has not been established.

By leveraging our well-established and multidisciplinary remote sensing expertise, Sandia is uniquely suited to address the uncertainties related to the utility of optical imaging polarimetry for remote sensing. Through a multi-faceted research approach, this project will investigate both instrument characterization and validation (through simulations and experimental data), as well as data exploitation and analysis. This work will also assess novel polarimetric data acquisition and processing technologies to provide a path towards the next-generation sensor architecture. The outcomes of this project will directly impact Sandia’s future national security missions in nuclear nonproliferation and other mission areas, and could provide the foundational research that establishes Sandia as a premier research center for optical polarimetric remote sensing.



## Exploiting Social Media Sensor Networks through Novel Data Fusion Techniques

191004 | Year 1 of 2 | Principal Investigator: T. M. Kouri

### Project Purpose:

National security is a major concern for the US, but it is becoming more difficult as threats continue to increase. It is imperative that we use every source of information available to assess and protect against the threats to our nation. Data is being generated at unprecedented rates, but is not being used effectively to exploit all of the information it contains. This data comes from a variety of sources, such as space, ground, and social media sensor networks, and these sources should be fused together to increase the amount of knowledge that can be gained from them. In addition to fusing data together from multiple sources, we must be aware of and look for potential misinformation in some of the data sources. Misinformation in data sources may be a result of sensor network impreciseness or a result of an adversary. Some data sources are more susceptible to providing misinformation than others. For example, we are much more likely to get misinformation from social media than from our own satellite ground stations.

Big data research has been ongoing for many years and there have been many significant technical advances recently, but there is still a lot of work to be done in order to fully exploit the knowledge contained in data sets. The development of new and efficient algorithms to fuse big data from multiple sources, which integrates existing techniques used in big data research with techniques developed during earlier research for automated reaction mapping are proposed.

This project proposes a challenging adaptation of applying techniques designed for automated reaction mapping to data fusion. If successful, the new algorithms will be able to efficiently integrate and fuse data from multiple sources, detect misinformation in sources, and exploit the resulting information.

## Exploring 2D Materials for Remote Sensing Applications

180836 | Year 2 of 2 | Principal Investigator: J. A. Bartz

### Project Purpose:

The purpose of the project was to create 2D heterostructure photodetectors with properties not realized through the use of bulk materials, in order to improve remote sensing capabilities. Density Functional Theory (DFT) was employed for material simulation throughout this project and has been used to identify 2D materials with electrically tunable optical absorption which would enable powerful adaptive and reconfigurable remote sensing applications.

In order to produce and characterize novel 2D material heterostructures, this research pursued three parallel approaches: modeling, flake-based heterostructure assembly, and chemical vapor deposition (CVD). Materials were modeled with density functional theory which provided insight and guidance. Next, this research aimed to create, characterize, and compare these 2D material heterostructures to the modeled results. Initially, this involved experimental verification of methods used to produce monolayers through mechanical exfoliation, including Raman Spectroscopy, photoluminescence measurements, and atomic force microscopy. Following production of micron-sized monolayers, heterostructure assembly was pursued. The third approach pursued large area production of monolayers through CVD. As this research focused on sensing applications, large area production of materials of interest was essential.

Infrastructure and experimental techniques were developed to address the challenges associated with micron-size devices. A laser scanning confocal microscope was developed for imaging as well as Raman and PL spectroscopy. This microscope enabled the identification of 2D materials. A digital widefield microscope was developed for real-time viewing of the exfoliation process. A characterization technique based on conductive tip atomic force microscopy was developed. This technique enables spectral characterization of 2D material devices without the need for lithography. Graphene CVD was successfully demonstrated and films were characterized. A new technique for CVD growth of black phosphorus was attempted. Strong photoluminescence was observed and the results are under investigation.





## FPGA Trust and Vulnerability Assessment Guided by Network Criticality Metrics

191011 | Year 1 of 2 | Principal Investigator: V. G. Kammler

### Project Purpose:

This research proposes a tiered, simulative, and formal modeling approach to analyze field programmable gate array (FPGA) designs implemented by untrusted vendor-provided software tools. Design input into these tools can be inspected and controlled, but design output, called an FPGA bitstream, is not as easily inspected. Functional equivalence can be checked, also by third party tools, yet there remain vulnerabilities that escape detection despite thorough benchtop testing. Existing methods for design trust often rely on a reference FPGA, ignoring the possibility that its bitstream has already been compromised. An assessor-based approach involves dedicating a highly technical team to recover functional behavior from each bitstream to confirm designer intent, a laborious and costly service repeated for each design version per FPGA device.

Complexity and design partitioning are often cited as the primary technical challenges for analysis of digital circuits including FPGAs. We investigated techniques that provide first-cut metrics that isolate regions of concern without prior knowledge of circuit function to scope the field of deeper analysis to a set of logic gates. We modeled the FPGA output as a Boolean network with nodes characterized by influence, a criticality metric based on Fourier transforms, to weigh downstream impact of activated logic. We combined these with published metrics that characterized the rarity of trigger before discriminating for intended function of the design. Statistics collected from simulations are then used to resolve for intended function and identify nodes that should receive greater scrutiny. In the next tier of analysis, we will apply property checkers to confirm the presence or absence of subversion. Test cases will include openly published trojans and internally developed designs of relevant complexity. If successful, the methodology can be expanded to include a broader range of not only commercial FPGAs, but application specific integrated circuits, all implemented using automated design tools, for the purpose of trust and vulnerability assessment.

## Flux: Toward a General Model of Moving Target Defense Efficacy

180831 | Year 2 of 2 | Principal Investigator: C. Lamb

### Project Purpose:

The concept of Moving Target Defense (MTD) is appealing because it promises to make our systems' attack surfaces less predictable to the adversary and, therefore, more resilient. However, few MTD approaches have gained acceptance in practice. In part, this is because many MTD approaches not only create less predictable attack surfaces, they also shroud system and network configurations, introducing additional complexity and cost for users, administrators, and defenders (i.e., they do not change the asymmetric nature of cyber attacks to favor the defenders instead). We propose to address this problem via a novel modeling approach highlighting the dependencies of complex systems and networks, from different perspectives, to highlight key exploitable differences. Such a representation provides deeper insight into the dependencies and needs of users, administrators, defenders, and attackers, allowing us to study the impact of MTD approaches on each set of agents. These different dependency representations, when compared, will allow us to identify and break attacker dependencies while preserving dependencies of legitimate stakeholders, leading to more resilient cyber systems potentially capable of dynamically adjusting to attacks.

In the first year, we focused on developing the initial model that we will then use to dynamically adjust cyber defenses in a running system. In the second year, we were able to demonstrate that our approach did, in fact, describe the way the address space layout randomization (ASLR) and related attacks evolved over time. We were able to show that ASLR defenses were initially strong against even determined adversaries, but that they were not effective without data execution prevention. We also used our approach to outline a way to use control theory to dynamically adjust the defensive posture of a given system. We were able to show that you can use state space models from control theory to model the dynamic interactions between attackers and defenders—and use that insight to dynamically select defenses with the highest possible effectiveness against a given attacker.



## High Fidelity ARM Virtualization for Large Scale Mobile Emulytics

180832 | Year 2 of 2 | Principal Investigator: D. J. Fritz

### Project Purpose:

With the rapid growth and availability of smart phones coupled with modern society's dependence on them, smart phones have become a prime target for cyber criminals and nation states. Smart phones are embedded in almost every facet of life, ranging from communication (calls, email, texting, and social-networking) to online banking, GPS navigation, and medical records. Government and industry both heavily rely on smart phones in the workforce and sensitive information of all kinds resides in them. The number of smart phones sold annually now exceeds the number of desktops and laptops combined.

This project adds a representative and large-scale ARM (Ashton Raggatt McDougall) architecture capability, as well as emulated sensors and radios for mobile devices, to Sandia's existing emulytics framework. ARM is the dominant processor architecture for smart phone and tablet devices, and is making headway into the laptop market. Existing platforms, both public and private (Amazon EC2, Sandia's minimega, Google Compute) currently only provide x86\_64 virtualization. While these platforms certainly provide performance and scale for desktop operating systems, they fail to provide an effective and realistic platform for mobile devices.

## High Fidelity Simulations of Large-Scale Wireless Networks

190979 | Year 1 of 2 | Principal Investigator: U. Onunkwo

### Project Purpose:

The worldwide proliferation of wireless connected devices continues to accelerate. There are tens of billions of wireless links across the planet, with an additional explosion of new wireless usage anticipated as the Internet of Things develops. Wireless technologies do not only provide convenience for mobile applications, but are also extremely cost-effective to deploy. Thus, this trend towards wireless connectivity will only continue, making it important to develop the necessary simulation technology to proactively analyze the associated emerging vulnerabilities.

Wireless networks are marked by mobility and proximity-based connectivity. The de facto standard for exploratory studies of wireless networks is discrete event simulations. However, the simulation of large scale wireless networks is extremely difficult due to prohibitively large turnaround time. A path forward is to expedite simulations with parallel discrete event simulation (PDES) techniques. The mobility and distance-based connectivity associated with wireless simulations, however, typically dooms PDES and fails to scale (e.g., OPNET and ns-3 simulators).

We propose a PDES-based tool aimed at reducing the communication overhead between processors. The proposed solution will use lightweight processes to dynamically distribute computation workload while mitigating communication overhead associated with synchronizations. Current research in large scale emulations have focused on wired networks, where two assumptions prevent scalable wireless studies: 1) the connections between objects are mostly static and 2) the nodes have fixed locations.

There is great uncertainty in the ability to use traditional computational systems to simulate large scale wireless networks. Mobility in wireless networks and the associated proximity-based communications makes such large scale simulations extremely difficult. The underlying problems with simulations in this field—process synchronization and load balancing—are unsolved, but yet the need for such investigative studies is ever increasing.



## Hybrid Classifiers Using Statistics and Machine Learning

190988 | Year 1 of 2 | Principal Investigator: K. M. Simonson

### Project Purpose:

The classification of unknown entities based on measured data is a fundamental challenge facing intelligence analysts, military commanders, and policy makers confronted with high-consequence decisions. Over the last decade, outputs from a wide range of sensors have provided a data-rich environment in which automated exploitation methods have begun to thrive. "Machine learning" techniques, including deep learning and support vector machines, offer the promise of fully or semi-automated classification of sensed scene or signal elements. While these methods have demonstrated some success on well-publicized data analytic challenge problems, they are susceptible to over-training, and generally fail to meet the performance standards required for critical applications. In addition, they are often viewed as opaque "black boxes," whose output is not understood or trusted by analysts and decision makers.

By contrast, Sandia has developed a novel approach to frequentist statistical classification, which allows complete traceability of all outputs, and provides rigorous consistency scores for gauging uncertainty. The method, known as Probabilistic Fusion (PF), has been applied to a range of mission-relevant classification problems, with successful operational transition to near-real time sensor feeds. However, training PF-based classifiers is a time-consuming and manual process, requiring considerable expertise in both statistics and sensor phenomenology.

Our research will focus on the development of a new family of hybrid algorithms and classifiers, which combine the ease of training associated with modern machine learning techniques, with the robust performance, transparency, and rigorous uncertainty characterization enabled by PF. The resulting classifiers will be applicable across a wide range of mission challenges.

The proposed research explores strategies for combining state-of-the-art machine learning techniques with Sandia's unique PF method. The goal is to develop an understanding of how to combine elements from each approach to build new hybrid classifiers that are practical, robust, and powerful. Successful execution will provide Sandia with a ground-breaking new capability that may have broad mission application.

## Hybrid Simulation-Optimization Methods for System of System Models

193420 | Year 1 of 1 | Principal Investigator: J. D. Siirola

### Project Purpose:

This project supported new research collaborations between Sandia's discrete optimization researchers and Purdue University's System-of-Systems (SoS) Laboratory. Purdue's SoS Laboratory is focused upon the development of foundational methods and tools for addressing problems characterized as SoS. They have developed SoS models like ARTEMIS, which can be used to evaluate, optimize value, and reduce risk of advanced missile defense concepts. ARTEMIS is focused on characterizing SoS integration risk—the risk that a step-change improvement in individual system technology (e.g., interceptor) is degraded (or even eliminated altogether) by emergent interactions in the larger SoS architecture. Hence, this capability provides an attractive platform for modeling how architectural and technological changes impact missile defense systems.

This project focused on identifying opportunities for new optimization approaches that couple with ARTEMIS when the space of alternatives becomes too large to support enumeration. This capability could support the use of ARTEMIS for large, complex missile defense design and analysis applications. Further, this capability reflects a characteristic that naturally arises in many national security missions: coupling of optimization methods with detailed simulation models. Thus, this research partnership catalyzed the integration of Purdue researchers into similar national security applications at Sandia.

Optimization of simulation-based models under uncertainty and frequently with multiple competing objectives is a critical capability for designing and operating complex engineered systems described by SoS models; however, even for modest-scale problems, there exist no generally accepted efficient numerical approaches. This project sought to explore several promising research ideas that would dramatically expand our ability to address these challenging problems.



## Hypersonic Autopilot Adaptive Control for Aerodynamic Uncertainty Mitigation

180826 | Year 2 of 2 | Principal Investigator: J. M. Parish

### Project Purpose:

Robust nonlinear control development for hypersonic flight applications remains a difficult, outstanding research problem. Uncertainties associated with large flight envelopes at extreme speeds make control design a particularly complex problem. The main drivers of system instability are aerodynamic uncertainties to which the vehicle is subjected throughout flight. Complicated aerodynamic phenomena such as shock-shock interaction, chemically reacting flow fields, hypersonic boundary layer transition, and surface ablation are difficult to predict through ground testing or computational simulations. Imprecise high altitude atmospheric models are additional uncertainty contributors. Flight test data provides discrete validation points for models, but the full continuum of the flight envelope is not well modeled and changes with mission objectives.

Adaptive control strategies have emerged in the aerospace community as potential solutions for handling these types of parametric uncertainties. Here, we proposed two adaptation strategies for parallel implementation with a dynamic inversion nonlinear controller. First, an augmentation variant of L1 adaptive control was developed to complement the nonlinear control strategy for a representative hypersonic vehicle. Recent L1 adaptive control developments offer significant advancements over past adaptive controllers with a new, strategic filtering architecture that permits significantly higher adaptation rates more suitable for agile hypersonic vehicles. Second, a center-of-mass (CM) mechanical adaptive control solution was investigated for providing a physical, real-time method for manipulating stability in the presence of large aerodynamic uncertainties. These two methods were evaluated for efficacy in face of aerodynamic uncertainties and for suitability for implementation on a flight test vehicle. These approaches build on past work by adapting the control signal, L1, or the vehicle itself, CM, to allow a nonlinear, model-based dynamic inversion controller to function more robustly.

## Hyperspectral Hypertemporal Database Reference Search Project

180845 | Year 2 of 3 | Principal Investigator: J. D. Zollweg

### Project Purpose:

We will advance explosives modeling, sensor design, and machine learning fields using a unified three-pronged approach.

The first aspect of this project is to create a cohesive and comprehensive database of events and signatures relevant to national security missions. This database will include fast transient data, such as high explosives (HE), artillery, and lightning as well as extended signatures like rocket plumes, tri-directional reflectance distribution function (TRDF) data, and backgrounds. Filling this database will require inclusion of advanced simulated data (HE signatures, TRDF hypercubes, etc.).

Modeling/simulation is the next area addressed by this project. Notably, we will partner with CRAFT Tech to develop a streamlined "HE-to-Photons" model. To advance the state of the art, and make simulated HE data practically feasible. The end result of this investigation will be a simplified workflow, with parametric inputs. This will enable filling of gaps in the assembled database and potentially even "modernization" of irreplaceable, but low resolution legacy data.

Finally, we will produce an end-to-end software tool called "Signals." Signals will simplify manipulation of high-dimensional datasets, enable research, and accelerate sensor/algorithm design workflows. There is currently no available tool that addresses this ambitious spectrum of goals. Everything from basic arithmetic of multidimensional signals, to phenomenology resources (radiometry, sensor/scenario modeling), and cutting-edge data exploitation (decomposition/factorization, target detection, classification) will be included. All together, Signals will be applicable to nearly any remote sensing problem. No existing software tool contains all of the diverse capabilities that Signals will. Signals will be closely integrated with the database constructed under this project, providing research not only with the most advanced remote sensing tools available, but also a wealth of curated legacy and simulated data.



## Imaging LIDAR and Raman Imaging LIDAR through Fog and Dust for Maritime Surveillance

173064 | Year 3 of 3 | Principal Investigator: S. A. Kemme

### Project Purpose:

This work supports Airborne Intelligence, Surveillance, and Reconnaissance for tactical situational awareness in challenging environments with modified imaging LIDAR (light detection and ranging). LIDAR produces an irradiance-based scene with high, 3D, spatial resolution; differentiating reflecting surfaces and surface textures not just for target detection, but also target recognition.

LIDAR is generally prevented from working through all weather—known as degraded visual environments—as the traditional source wavelengths are scattered and/or absorbed by fog, clouds, and dust. This work identifies and quantifies improved optical wavelength regimes and polarization strategies that should open this otherwise denied operating window for LIDAR. Other research has identified singular and limited wavelengths that are optimized for range; here we identify broad wavebands where range is extended. Similarly, previous researchers have utilized linear polarization to improve range. In contrast, we show that circular polarization is frequently the optimal choice for many wavelength regimes in scattering environments. We demonstrate modified imaging LIDAR's utility and ability to produce images in environments that have been challenging for traditional LIDAR (fog, dust) systems.

## Imaging Mass Spectrometry for Biometric and Forensic Detection

173069 | Year 3 of 3 | Principal Investigator: J. M. Hochrein

### Project Purpose:

There is a significant need to unambiguously determine a person's identity and locations where he/she has been. Traditional biometric approaches such as fingerprinting, hair analysis, DNA, and retina/iris scanning typically target one characteristic and often require previous knowledge of the individual. We propose using imaging mass spectrometry to identify new biometric signatures addressing several characteristics simultaneously and generating a fingerprint map. High-resolution mass spectrometry combined with imaging is a highly versatile tool applicable to many analytes including small molecules, semi-volatile, and non-volatile species including biomolecules. This technique has been demonstrated on explosive residues, drugs of abuse, inks, and many other organics. In most cases, complex matrices have not been investigated. Specific markers that would be of interest to identify not only a specific person or group of people but also provide information on their activities or working environment remain to be characterized. This research will focus on the discovery of new chemical markers from fingerprints and other biological targets including hair, nails, skin, ear wax, and saliva that will be used to identify biological and environmental signatures unique to an individual or group of people of interest. Significant advances have been made to enable the positive identification of people based on biometric signatures but many of these techniques require considerable knowledge of the person prior to identification. Additionally, some of the biometric signatures can be manipulated rendering them ineffective or ambiguous. The focus of this work will be to identify several new key signatures while at the same time generating a high-resolution image, making identifications much higher fidelity.





## Implementing Neural Adaptive Filtering in Detection Systems

190993 | Year 1 of 3 | Principal Investigator: F. S. Chance

### Project Purpose:

A major challenge facing detection systems is detecting signals-of-interest in noisy backgrounds. The difficulty of this task is amplified by increases in sensor sensitivity and the addition of multiple sensor modalities into the detection system. Modern detection systems must, therefore, have the capability to handle an ever-increasing diversity of “clutter” or “distractor” signals. Current state-of-the-art solutions implement noise-cancelling filters with fixed parameters. Although fast, these do not protect against more complex adversarial distractor signals. The goal of this project is to develop novel neural-inspired adaptive filtering algorithms that operate at the sensor level. We envision that this algorithm will be useful in a variety of detection systems, including those using state-of-the-art multimodal sensor arrays, processing hyperspectral data, or relying on remote sensors (with limited bandwidth of signal transmission to the processing platform).

Our research will focus on understanding the algorithms employed by the retina (the sensor of the visual system) to adaptively filter visual information. In particular, we will focus on developing novel algorithms inspired by the functions of retinal ganglion cells (the output cells of the retina) and on elucidating novel implementation strategies (based on the circuitry of the retina) of in-use algorithms modern detection systems. While retinal circuitry may appear simple compared to higher-level areas of the brain, recent advances in neuroscience methodologies have revealed a surprising diversity of retinal cell types (detecting motion, color, etc.) that perform an equally wide range of computations to “preprocess” visual input for transmission through the information bottleneck of the optic nerve (en route to the brain). We propose that strategic modifications of these algorithms will enhance the performance of detection systems by allowing them to filter a range of distractor signals, potentially at the sensor-hardware location, leaving more bandwidth for transmitting signals-of-interest.

## Improving Radiation Spectra Identification for Radioactive Materials with Uncertain Configurations

180846 | Year 2 of 2 | Principal Investigator: M. L. Koudelka

### Project Purpose:

Sandia is a leading developer of spectroscopic radiation detection systems and a leading source of expertise in analysis of gamma-radiation signatures. Due to the demanding environments in which these radiation detection systems are required to operate, data is often of poor statistical quality. In the most challenging scenarios, radioactive sources are highly shielded and the data collection time is short, leading to smooth and nearly featureless spectroscopic signatures. Current signature identification techniques involve fitting computed spectral signature exemplars to measured data of interest to determine the radiation source. These methods generally require high fidelity data as well as highly knowledgeable individuals to guide the analysis by intelligently selecting and computing exemplars to match against radiation signatures of interest. Improved methods are needed to further the state of the art for the rapid assessment of gamma-ray signatures with uncertain configurations. We proposed the development of algorithms and techniques that can capture the variability in radiation spectra across an array of possible configurations with a limited set of template-based representations.

We have leveraged target identification algorithms developed at Sandia and currently employed for radar signature identification. In doing so, we addressed issues related to variable shielding, as well as varying data quality. We expanded upon the initial research question to explore the possibility of identifying additional variables related to the sources under test.

The goal of the proposed research is to improve Sandia’s capability to identify radioactive materials using low fidelity gamma radiation spectra, where the configuration of the radioactive object is unknown. This research is risky, yet has the potential to produce a significant advancement in the state of the art analysis of gamma radiation spectra.



## Inferential and Feature Selection Methods for Video Imaging

190980 | Year 1 of 2 | Principal Investigator: M. G. Chen

### Project Purpose:

With the rise of electronic and high-dimensional data, new and innovative statistical methods are required to perform accurate and meaningful statistical analysis of these datasets that provide unique statistical challenges. Data dimension reduction and inference facilitate statistical analysis that may identify changes or anomalies in large populations of data. While high-dimensional data analysis has been a main focus of recent statistical methodological research, much focus has been on populations of high-dimensional vectors, rather than populations of high-dimensional matrices. There are many sources of data that contain multiple high-dimensional matrices, such as synthetic aperture radar and coherent change detection video images, brain imaging, and financial data, among many examples. While some methods for dimension reduction and inference have been developed purely from a mathematical standpoint, these methods may not be applicable to many real datasets due to their assumption that all observations in a given population are independent and identically distributed. This project seeks to develop new inference methods to identify changes or anomalies in a population of images obtained from dependent observations. Once these differences have been identified, we will characterize and extract the features through unsupervised methods that can detect features that could be previously unknown. This is in contrast to recently used methods, such as deep learning and neural network methods, that require a training set to perform supervised learning. Methods developed will be applied to optical video data of passing train cars, and performance of methods will be evaluated on the ability to detect distinguishing train car design features found in the video.

## Intelligent Control for Autonomous Penetration (ICAP)

180825 | Year 2 of 2 | Principal Investigator: S. Buerger

### Project Purpose:

The purpose of the project is to research the application of advanced feedback control to improve the performance and autonomy of select nonkinetic penetration technologies. The present state of the art requires expert human operators to manually operate most relevant nonkinetic penetration systems, exploring system settings, and working to optimize performance via a combination of learned expertise and trial and error. The operator makes adjustments at arbitrary intervals to maximize performance (e.g., rate of penetration and energy efficiency) and to manage disturbances such as variations and transitions in material properties. Recent advances in sensors, control systems technology, and penetration capabilities make it possible to develop novel intelligent penetration systems that adapt in real time to reject disturbances and optimize performance without operator intervention. This project developed and demonstrated intelligent penetration systems. Work includes a combination of modeling, control system analysis and design, and experimentation. Models of penetration processes were developed and parameterized through experiments conducted at existing specialized Sandia test facilities, which were outfitted with additional instrumentation. Controllers will be designed in simulation and tested experimentally. The project culminated in "one-touch" demonstrations, in which a prototype system autonomously penetrated a multi-layer sample with a single operator command. Performance was shown to significantly exceed that capable with any single, open-loop system setting.



## Internal Structure Mapping with X-Ray Phase Contrast Imaging

180838 | Year 2 of 2 | Principal Investigator: A. L. Dagele

### Project Purpose:

The purpose of the project was to investigate a capability that would enable nondestructive imaging of low density materials. Authenticity and verification of commercial components used in trusted electronics is a complex process of procurements and inspections. It is critical that inspection methods effectively identify material, process, or mechanical variations between procurements. Current effective methods are destructive in nature and employ "slice and dice" inspection of randomly selected samples. Less effective nondestructive methods are limited in imaging depth, require complicated sample preparation, and are limited in materials that can be inspected. x-ray absorption imaging is currently used for nondestructive imaging; however, it has poor sensitivity to low absorbing (low-Z) materials.

X-ray phase contrast imaging (XPCI) enables imaging of low density materials and produces three complementary image products, and therefore, greater information about the sample. In all materials, the phase coefficient is larger than the absorption coefficient, resulting in much higher contrast in phase-based imaging than traditional absorption imaging. For low-Z materials, the difference between coefficients is three orders of magnitude. The increase in contrast sensitivity can be employed for imaging multi-material stacks where neighboring materials have small changes in density. One of the keys to making XPCI successful is large area, high aspect ratio x-ray gratings with high uniformity. Sandia has a world class capability in the fabrication of the challenging gratings that enable the XPCI technique. There are few other XPCI systems around the world, none has large area gratings with comparable uniformity, few are studying materials science applications, and we are able to leverage unique knowledge in image reconstruction and phase unwrapping employed in other applications at Sandia to reconstruct challenging samples. XPCI is an important nondestructive imaging modality with the potential to impact a broad range of applications relevant to national security.

## Low-Power Sensor Authentication using Public PUFs

195218 | Year 1 of 1 | Principal Investigator: J. Hamlet

### Project Purpose:

Physical unclonable functions (PUFs) in integrated circuits are typically multiple-input, multiple-output measurements of uncontrolled manufacturing variations that are easy to measure but hard to predict. This makes PUFs useful for authentication and cryptovariable generation. It is established that PUF-based cryptographic authentication of sensor data can provide extremely robust authentication, but the complexity of the measurements and cryptographic operations requires a relatively large amount of power (computational and electrical) that can render a traditional PUF unusable for remote operations. Public PUFs (PPUFs) are a new form of PUF that offers fast evaluation at low power. With PPUFs, simulation of the output appears feasible but time consuming. However, the PPUF approach uses response time to a challenge as a metric that contributes to verification of authenticity. Direct measurement of PPUFs is fast, while playing back a spoofed response is relatively slow and an indicator of an attempted subversion. Using PPUFs, security protocols have been proposed but these techniques are so new that many questions remain concerning their practicality and potential vulnerabilities. For instance, PPUF approaches provide authentication, but they are not truly unclonable and they do not appear to provide the inherent tamper evidence of cryptographic PUF authentication. This project is to prototype an efficient cryptographic PPUF-based approach for authentication of remote sensors and to compare the approach to traditional cryptographic authentication approaches with respect to area, speed, and power consumption. Efforts to develop PPUFs for sensors may be extensible to other scenarios, such as network access control.



## Macro Supply Chain Decision Analytics

180859 | Year 2 of 2 | Principal Investigator: R. Helinski

### Project Purpose:

Today's global supply chains are intrinsically complex systems that make security and integrity risk difficult to manage. The US Government Accountability Office (GAO) reports that many US Government agencies lack sufficient capabilities to address global supply chain security risks [GAO-12-361, National Security-Related Agencies Need to Better Address Risks, p.18]. No analytic tools exist that assist decision makers in capturing, visualizing, and assessing the state of health of a supply chain holistically. A National Institute of Standards and Technology (NIST) Special Report explicitly calls out the importance of holistic supply chain metrics: visibility and traceability. Complex corporate structures and distribution networks reduce these properties, making it extremely difficult to secure the supply chain of an end product. Furthermore, the ownership of corporate structures can change overnight; hence, understanding a supply chain is a continuous process. As a result of these factors, it is difficult to understand supply chain risk and decide where to gather more information or apply mitigations.

The purpose of this project is to develop analytic methods to construct a bird's-eye view of a production process and its associated supply chains, and to identify and assess macro-level indicators to help policy and decision makers make better decisions. We created a framework that can be used to represent a supply chain at a high level, using a top-down approach that mitigates the depth of the supply chain. Risk assessment, based on seven high-level risk indicators, is performed on our representation, evaluating touch-points and dependencies. The result of this risk assessment indicates specific areas that might need a deeper investigation.

Previous supply chain risk management research focused on analysis of suppliers and commercial-off-the-shelf alternatives, or only dealt with cyber security issues. Instead, our framework enables an enterprise-level analysis of a business process that generates some end product, including all of the people, organizations, materials, information, and interactions with external parties that are involved.

## Measurement of the Optical Opacity of Warm Dense Gas Mixtures to Support High Fidelity Modeling and Interpretation of the Optical and Thermal Emission from Conventional and Nuclear Fireballs

191001 | Year 1 of 2 | Principal Investigator: P. L. Dreike

### Project Purpose:

We are developing experimental procedures to make low uncertainty measurements of the spectral opacity of "warm" (4000K to 12,000K) gas mixtures (initially air) from one-tenth to ten times standard density. This data is needed to model optical emission from conventional explosive and nuclear fireballs (NUDETs) in order to understand the physics of chemical explosions and determine NUDET yields. Opacity of explosion products governs their light emission. NUDET yields are related to their fireballs' optical emission history, which depends on the transition of an air shock from being optically thick to optically thin as the cooling air opacity decreases. The only existing air opacity data consists of legacy theoretical air opacity tables (ca. mid-1970s) that lack known controlled experimental validation.

Contemporary studies of emission from conventional explosions, higher spectral resolution NUDET optical models to support sensor design, and UQ of model-based NUDET yield determination are handicapped by these opacity table limitations. Because fireball temperatures exceed solids' vaporization temperatures, opacity measurements must be dynamic. We proposed using a two-stage light gas gun to: 1) shock gas in a "gas-cell" to appropriate temperatures and densities and then 2) accurately measure the time-resolved spectral emissions that are proportional to gas opacity. To support the experiments, calculations using legacy air opacity tables identified the most important temperature, density, and spectral ranges for opacity measurements to support NUDET optical modeling. The first target design tested directly shocks a platinum target that in turn shocks air in a gas cell. Although our modeling predicted a 1900K platinum temperature with thermal emission smaller than the shocked gas emission, platinum emission was brighter than the expected gas emission. A second target was designed that uses "quasi-isentropic compression" to launch a cooler copper target into the gas. The measured copper velocity history was similar to the predicted history and a sensitive photodiode detected no thermal emission.



## Meta-Meta-Optimization for Integrated Requirements Development

180855 | Year 2 of 2 | Principal Investigator: A. Dessanti

### Project Purpose:

Early in government acquisition programs, a highly complex and interdependent set of requirements is developed. These requirements define what the system being procured must do, typically with threshold (minimum desired) and objective (desired if possible) values for each requirement. Requirements are usually derived from user needs and each possesses strong rationale and analytical backing for why the threshold and objective values were set as they were.

Groups of requirements (such as mobility or survivability requirements for a combat vehicle), however, are generally developed by independent teams of Subject Matter Experts who have a thorough understanding for their area of expertise. When all the individual requirements are integrated into a single set that the system being procured must meet, inconsistencies or unaffordable scenarios sometimes arise. If these issues are not addressed early, they can present challenges to a program down the road and ultimately contribute to programs being cancelled or delayed. Traditionally, this integration process is performed manually through negotiations between the relevant stakeholders.

An analytic capability to support integration of individual requirements into a simultaneously achievable set while considering programmatic and technological constraints would reduce the risk of inconsistent or unaffordable sets of requirements persisting beyond the early stages of a program. This capability would also help bring some of the analytic support that the individual requirements have to the integration negotiation process, making it easier to defend decisions that are made. The capability developed during this research project, which was enabled by algorithmic advancements in ultra-high dimensional optimization, provides this unique analytic support.

This concept is novel within the optimization literature and will likely lead to new industry standards for ultra-high dimensional optimization. It will keep Sandia on the cutting edge of robust analytics for acquisition programs, with applications not only for the military, but also broader application spaces including the nuclear weapons enterprise.

## Microsystems Enabled Passive RF Signal Processing

190996 | Year 1 of 2 | Principal Investigator: C. Nordquist

### Project Purpose:

Resonant radio frequency (RF) microelectromechanical systems (MEMS) can perform passive signal processing and signal discrimination to enable low- or zero-power receivers for future networking concepts such as the "Internet of Things." The frequency selectivity and passive voltage gain in piezoelectric focusing transducers coupled with the mechanical resonance and high threshold slope of a MEMS switch enables signal selectivity to both the center RF frequency and modulation, with added benefits of energy integration and a high on/off ratio. The project goals are to demonstrate an RF MEMS resonant wake-up system, understand future paths to improving performance, and identify application opportunities. Research topics required to achieve these goals include: understanding the system design factors that influence the sensitivity and selectivity of the microsystem, optimizing the individual devices for maximum performance, and fabrication and integration of the devices for optimum performance.

This project extends previous RF microsystem work in several directions and has resulted in several new developments. First, closure of a MEMS switch with a resonant RF envelope drive had not been demonstrated prior to this project. Second, a biased resonant switch presents nonlinear dynamics that had not been explored previously. Third, obtaining maximum sensitivity in a resonant MEMS switch requires optimization of different parameters than for a traditional RF MEMS switch. Fourth, focusing transducers have not been demonstrated as impedance transformers for passive voltage gain. Finally, intimate integration of the two different components is required for the best performance.

In the first year of the project, we have fabricated aluminum nitride resonant transformers with passive voltage gain, fabricated resonant RF switches with  $Q > 1000$ , performed modeling and experiments to determine the best waveform modulation for minimizing closure energy, and demonstrated closure of a MEMS switch with modulated RF drive. Future work will focus on using better materials to improve the passive voltage gain and switch  $Q$ , which will improve sensitivity.





## Motion and Trajectory Algorithms for Visual Information Foraging in Intelligence Analysis Workflows

193424 | Year 1 of 3 | Principal Investigator: L. A. McNamara

### Project Purpose:

This project is producing data, algorithms, and prototype software that enables researchers to infer visual problem solving strategies from gaze data collected as human searchers (analysts) interact freely with imagery data. Although eye tracking systems have practical application across a wide range of domains, they are not designed for capturing gaze events in the dynamic, user controlled foraging workflows that constitute real-world imagery analysis “in the wild.” This is because eye tracking systems capture gaze samples against the (x, y) plane of a display, rather than in relation to the content of the display. If stimuli are static, mapping gaze events to pixelated content is straightforward. However, mapping gaze events to image content is quite difficult when users are unpredictably manipulating an image as they look for features of interest (i.e., by panning, changing resolution, adjusting luminance contrast, or other presentation parameters). This limits the utility of eye tracking to diagnose human performance issues in real-world softcopy search tasks.

In FY 2016, we developed a stimulus presentation and gaze data collection system based on the commercially available Fovio eye tracker, to automatically correlate gaze events to content, rather than screen coordinates. The system uses geospatial synthetic aperture radar (SAR) imagery in which every pixel is georegistered, which facilitates the transformation of gaze samples collected in display space into gaze events that can be expressed as geocoordinate locations. Empirical evaluation consisted of human participants performing highly curated “search” tasks that mimic basic workflow elements in realistic imagery analysis environments (flickering between images, panning an image). This work is the foundation for a series of FY 2017 development iterations in which we will progressively expand the classes of visual interaction behavior, gaze events, and image types; and develop a verification and validation framework to assess the development state of our system.

## Multimodal Data Integration Under Uncertainty

190991 | Year 1 of 3 | Principal Investigator: D. J. Straczuzzi

### Project Purpose:

We will develop methods for estimating the uncertainty generated by the integration of multiple sensor modalities. The goal is to improve information extraction in multisensor settings by evaluating the uncertainty in the data. As the analysis of remote sensor data becomes increasingly automated, with human decision makers becoming increasingly removed from the raw data, we assert that uncertainty analysis must play an increasing role in data analytics. Our hypothesis is that uncertainty captures nuanced information about the data and associated decisions that cannot be replicated elsewhere. Although myriad integration approaches have been developed over the past several decades, most are specialized to sensor combinations, domains, and tasks. Relatively few of these provide a rigorous evaluation of the uncertainty associated with identified targets, which leaves them with little or no way to quantify the uncertainty in, and therefore justify, their conclusions. We also differentiate from the common practice of measuring the probability of detection and false alarm, and then using receiver-operating characteristics as a proxy for the “uncertainty” associated with the detection algorithm.

We ground our efforts in mission-relevant data, focusing on tasks and domains for which several different data sources are available. Combinations of three or four sensors let us identify and address issues in generalizing the uncertainty estimation methods. Key research tasks include:

1. Developing methods for unsupervised, probabilistic segmentation of single data sources that provide full posterior probability distributions.
2. Developing methods for marginalizing over multiple single-source segmentations using supervised data.
3. Developing methods for visualizing both confusion among class assignments and uncertainty in the probability distributions.
4. Evaluating the relative contribution of each data source to the final result.

If successful, our methods will produce the probabilistic distributions needed to support uncertainty quantification throughout analytic process, from collection to decision making.



## Multitarget-Multisensor Tracking

190999 | Year 1 of 2 | Principal Investigator: R. H. Byrne

### Project Purpose:

The goal of this research will be to apply finite-set statistics (FISST), which were introduced in the mid 1990s, to develop Bayesian multitarget multisource tracking and fusion algorithms for national security applications, particularly those in remote sensing. The basic concept of finite-set statistics is to mathematically transform the multisensor-multitarget problem into a single-sensor single target problem. This is accomplished by bundling all sensors into a single "meta-sensor" and all targets into a single "meta-target." A benefit of FISST is that it easily incorporates data from different types of sensors, including English language statements, into a common mathematical framework (a random subset) for common processing. By incorporating random set methods, it is also possible to include many expert system methodologies in a unified framework (e.g., fuzzy logic, the Dempster-Shafer theory, rule-based evidence, etc.). Natural language statements can be easily incorporated via fuzzy membership functions. While not the focus of this research, the ability to fuse natural language statements with sensor observations is attractive for some applications. A difficulty with other Bayesian formulations is that the number of targets, and the number of target states must be known in advance. Using FISST, the two conflicting processes of target detection and target estimation are estimated jointly, obviating the need to select the number of targets or state structure in advance.

## Novel Materials and Devices for Solid-State Neutron Detection

176117 | Year 3 of 3 | Principal Investigator: K. B. Pfeifer

### Project Purpose:

Neutron sensing is critical in civilian, military, industrial, biological, medical, basic research, and environmental applications. Conventional neutron sensors are limited by size, weight, cost, portability, and helium supply. Here the microfabrication of Gd conversion material-based heterojunction diodes is described for detecting thermal neutrons using electrical signals produced by internal conversion electrons (ICE). Films with negligible stress were produced at the tensile-compressive crossover point, enabling Gd coatings of any desired thickness by controlling the radiofrequency sputtering power and using the zero-point near  $p(\text{Ar})$  of 50 mTorr at 100 W. Post-deposition Gd oxidation-induced spallation was eliminated by growing a residual stress-free 50 nm neodymium-doped aluminum cap layer atop Gd. Resultant coatings were stable for at least six years, demonstrating excellent product shelf life. Depositing Gd on the diode surface eliminated air gap, leading to improved efficiency and facilitating monolithic microfabrication. The conversion electron spectrum was dominated by ICE with energies of 72, 132, and 174 keV. Results were reported on neutron reflection and moderation by polyethylene for enhanced sensitivity and  $\gamma$ - and x-ray elimination for improved specificity. Optimal Gd thickness was 10.4  $\mu\text{m}$  with 300  $\mu\text{m}$  thick partially depleted diode of 300  $\text{mm}^2$  active surface area. Fast detection within 10 minutes at a neutron source-to-diode distance of 11.7 cm was achieved using this configuration. All ICE energies along with  $\gamma$ -ray and  $\text{K}\alpha$  x-ray were modeled to emphasize correlations between experiment and theory and to calculate efficiencies. Semiconductor thermal neutron detectors offer advantages for field sensing of radioactive neutron sources.



## Novel Techniques for Silicon Doping Profiling

191013 | Year 1 of 1 | Principal Investigator: J. J. Sniegowski

### Project Purpose:

Nanoscale characterization of dopant distributions is important for integrated circuit technology. This problem becomes significantly more difficult as device dimensions shrink particularly for sub-22nm technology nodes. The helium ion microscope (HeIM) is a relatively new technology that has attracted great attention due to its ultrahigh resolution imaging capability, which has been shown to outperform the scanning electron microscope (SEM) in certain applications. The intent of this project was to explore the use of the HeIM for dopant mapping as related to silicon microelectronics. This project took two separate approaches: 1) imaging using the secondary electron signal, which is the conventional use of the HeIM and 2) a novel approach that attempted to convert a dopant distribution into a measurable topographical and preferably concomitant secondary electron signal.

Bare silicon with a range of dopant concentrations and large micron-scale test structures with varying dopant concentrations were studied in order to simplify sample preparation and analysis/interpretation of results. The secondary electron imaging was performed over the full available parameter space of the instrument. Various surface treatments were also explored in an attempt to maximize the effectiveness of the contrast mechanism.

## Novel, Semi-Destructive FA Technique for Stacked Die

173039 | Year 3 of 3 | Principal Investigator: R. J. Shul

### Project Purpose:

Stacked die for 3-dimensional integration (3-DI) are rapidly becoming a reality for commercial applications. The technology utilizes through silicon vias (TSVs). From a failure analysis (FA) perspective, 3-DI presents many challenges because the die of interest can be obstructed by other stacked die and are extremely thin and fragile. Destructive preparation techniques where the die are separated to access internal components fail due to loss of device functionality. Thus, there is an emerging demand for an innovative, semi-destructive process to access and connect to targeted TSVs or solder bumps on 3-DI devices that are sandwiched between the stacked die and are not accessible from the large faces of the die stack.

We investigated semi-destructive micromachining of Si substrates from the edge of a die to access connections to device circuitry, via the TSVs that connect the stacked die. With this novel approach, we evaluated micromachining techniques including plasma etch, selective vapor-phase etching, and gas-assisted laser ablation. Dielectric and metal atomic layer deposition (ALD) were investigated for making low-resistivity connections through etched holes. Initially, outer rows of TSVs were targeted for micromachining. Ensuing work extended the aspect ratio for both the skeletal and targeted single-hole micromachining and subsequent ALD to determine how deep connections can penetrate a die.

To our knowledge, this is the first attempt to remove material from the edge of a die for targeted drilling and connection to buried conductors while retaining device functionality. In addition to being the first semi-destructive FA approach to 3-DI, this work is revolutionary in at least three respects: 1) plasma etching of a die on edge has not been attempted and will require unique fixturing and masking, 2) chemical-assisted laser ablation to create high aspect ratio holes has not been implemented for edge approach, and 3) ALD into high aspect ratio drilled holes has not been utilized for FA.



## Patterns of Life Algorithm Development Via Semantic Graphs

190976 | Year 1 of 2 | Principal Investigator: S. J. Bussell

### Project Purpose:

This research will use spatiotemporal semantic graph algorithms and statistics-based modeling techniques to represent the operations tempo for a region of interest. This is a difficult problem given the high volume of data and complexity of algorithms required to establish these wide-area patterns of life. Addressing this problem requires: 1) developing new ways of using spatiotemporal semantic graph techniques to formulate algorithm designs that can detect and correlate anomalous activities over time and find hidden relationships among entities of interest and 2) involves statistical models/algorithms applied over wide areas where activities/relationships of interest are not well known.

As a high level notional example, suppose the spatiotemporal semantic graph algorithms detect correlation in activity between Hotel H and Location L. Also suppose that the function of Hotel H is well known (high-end accommodations for wealthy clientele), but the function of Location L has not to date been characterized. The semantic graph algorithms, by correlating activity between locations, can potentially be used to characterize the function of Location L (possibly related to high-end services). Thus, this solution, if successful, will provide a pathfinder for analytical tools that highlight anomalous activity/discover hidden relationships over wide areas and across multiple functional domains spanning many national security disciplines.

## Pinned Photodiode Pixel Development Enabling High Performance Visible FPAs

180841 | Year 2 of 3 | Principal Investigator: R. R. Kay

### Project Purpose:

Commercial technology has advanced state of the art in visible focal plane arrays to pixel sizes of about 1 square micron, while implementing pinned photodiodes to reduce dark current and noise. Pinned photodiodes have been proven to drastically reduce the contribution to dark current from surface states. However, no consideration has been given to other attributes important to national security remote sensing missions; namely, ultra-wide dynamic range control, radiation hardness, and on-shore availability.

This work focuses on developing pinned photodiode intellectual property for an on-shore foundry, nominally Sandia's CMOS7 process, and to fabricate and test small focal plane arrays to demonstrate pixel performance. If successful, the capability developed in this project, and the risk buy-down associated with its development, are anticipated to benefit numerous national security programs, particularly in the development of large format arrays utilizing the technology.

Devices fabricated during the first year of the project have been tested for leakage current, charge-to-voltage conversion gain, spectral quantum efficiency, and operation of a dual-gate approach to nondestructive read. Additionally, compatibility with baseline transistors has been verified.

Leakage currents of the best pinned photodiodes measured are approximately  $1\text{E}-11$  amps per square centimeter at room temperature. This is comparable to reported commercial devices. Conversion gains were measured to be about 9 microvolts per electron. This is about a factor of 5 below anticipated values, primarily due to high parasitic capacitance on the sense node of the device. A number of lessons learned from testing first-generation devices have been incorporated into second-generation devices that are presently in fabrication.

The dual-gate devices show operation as intended. The two gates can be used as row and column selects in focal plane arrays, and the amount of accumulated charge can be tested by varying the applied transfer gate voltage. This characteristic shows promise that the pixels can be used for wide dynamic range extension.



## Plasmonic-Based Optical Modulators and Switches

173490 | Year 3 of 3 | Principal Investigator: W. F. Seng

### Project Purpose:

Traditional interconnect wiring at the chip level is too slow and not able to carry the massive amounts of information required by "Big Data." Optical fibers and photonic circuits can handle the data, but their components are currently too large to be integrated at the chip level to merge with electronics. Surface plasmon-based circuitry is the key way to integrate electronics with photonics at the nanoscale for chip level application, achieving a circuit that can carry both electrical current and optical signals.

Exploring nanoscale device structures offering the possibility to achieve sub-wavelength mode volumes will result in previously unattainable light-matter interactions. Therefore, such efforts offer truly unique opportunities for switching/modulation and wave mixing applications, and devices operating based on this approach are anticipated to greatly surpass the performance of the current state of the art in speed, size, loss, and efficiency. These devices have direct application in optical networking and in creation of chemical and biological sensors that will fuel future growth in health and energy industries.

The work is in collaboration with UCLA.

Current photonic sensors, switches, and mixers are constrained in frequency response and overall SWaP requirements. A new approach is needed offering the possibility to achieve sub-wavelength mode volumes resulting in previously unattainable light-matter interactions. The project utilizes a necessary cross-pollinating combination of groundbreaking materials science with semiconductor fabrication uniting electrical and optical device characterization work.

Recent progress in this research has led to development of MiBo (modulation index boosting) as a key component to increase both low and high frequency sensitivity while reducing electrooptical modulator drive voltage  $V_{\pi}$  by a factor of 50, especially useful for multichannel wide bandwidth high energy pulse diagnostics.

## Quantifying the Uncertainty of Risk Assessment for High Consequence Flight Tests

173070 | Year 3 of 3 | Principal Investigator: T. M. Jordan-Culler

### Project Purpose:

High consequence flight tests for national security applications require review and approval of the risks associated with any flight program involving Sandia personnel or assets. Support of these reviews must deliver quantified risk uncertainties to decision makers. The Range Commanders' Council 321-10 Standard has provided guidelines for uncertainty quantification in probabilistic risk assessments. The Department of Defense continues to fly increasingly more complex flight tests that will be better designed when informed about uncertainties. This project investigated novel techniques of incorporating uncertainty into the current Sandia range safety probabilistic assessment tool, PREDICT, without significantly increasing computer run time.

Risk analysis is a process dependent upon mathematical models with many parameters used to simulate the consequences of vehicle failures, containing approximations used to describe debris, trajectories, motor and component malfunctions, and population or asset demographics. The models are approximations at various levels of sophistication and the model parameters are frequently difficult to quantify accurately. The goal of this research was to assess the epistemic uncertainty in predicted flight test risks, specifically by incorporating "uncertainty on the uncertainty" into the calculations.

Several different probabilistic risk assessment tools exist at the national ranges for flight safety analyses. None currently contain clear-cut methods for calculation of uncertainty quantification or confidence bounds on the predictive risk calculations. An uncertainty quantification approach to calculating epistemic uncertainty was delivered to PREDICT, building on the capabilities of DAKOTA (Design and Analysis toolKit for Optimization and Terascale Applications), which was developed through the fundamental research of DOE's Advanced Simulation and Computing program. The uncertainty quantification methods were customized and tailored for PREDICT's application needs. This research performed an additional level of uncertainty analysis, so that analyses now result in an ensemble set of predicted risks, from which the mean and standard deviation are calculated.





## RF Enabled Cyber: Incorporating RF Channel Effects in Modeling of Wireless Networked Information Systems

190992 | Year 1 of 2 | Principal Investigator: B. P. Van Leeuwen

### Project Purpose:

Wireless networking is increasing around the world and in all sectors of our lives. Wireless connectivity is integral to mobile communications for many of our nation's military and defense systems, smartphones, and low-cost deployments in the Internet of Things. Critical infrastructure systems are benefiting from significant increases in sensors and smart meters that report data via wireless communications. Systems that employ wireless connectivity must be evaluated under conditions that represent realistic wireless radio frequency (RF) channels, spectrum use, and protocol interactions.

Cyber researchers evaluating information systems, supporting protocols, and applications that benefit from testbeds capable of high-fidelity modeling. Testbeds used today are comprised of real, emulated, and simulated devices and/or subsystems and are primarily focused on wired systems. Wireless systems and their unique operation characteristics are much more difficult to represent in testbeds and/or modeling environments. Operational wireless systems use RF spectrum, licensed and unlicensed, to transmit data. For test and evaluation purposes, it is undesirable or prohibitive to emit energy into the RF spectrum. Researchers seek capability to test and evaluate wireless systems without emitting RF energy.

We propose a research effort to develop unique capability to represent wireless channel effects and wireless protocol interoperability when modeling wireless networked systems. Our research is creating methods to model wireless network protocols and protocol interactions, at both the data plane and control plane. Additionally, RF interference resulting from multiple-system waveforms and intentional interference resulting from RF jamming of the spectrum will be modeled. System fidelity will be further increased by incorporating the necessary physical layer and media access control layer protocols, interactions with upper layer protocols, and environment effects.

The research is advancing cyber analysis-platform modeling technologies and will provide a novel capability for the analysis of RF-enabled cyber impacts on wireless networks. The research will advance our cyber analysis capability to assess impacts to critical wireless systems by cyber manipulation of protocols and applications via the wireless channel.

## Realistic Internet of Things (IoT) Signal Control

190978 | Year 1 of 2 | Principal Investigator: I. Zedalis

### Project Purpose:

The purpose of this project is to address what we, as defenders, can do to obfuscate or disrupt an adversary's ability to use Wi-Fi-based IoT (Internet of Things) devices to monitor ambient, encrypted Wi-Fi traffic, and infer a variety of information about the network and the building in which the network is physically present.

Currently, all indications are that the IoT market will continue to grow as time goes on, slowly eating away at the market share of wired technologies. An example of this is how it is becoming more and more difficult to purchase a printer or a scanner that does not have a Wi-Fi interface. Furthermore, modern anti-tamper and integrated design methodologies have created a situation where Wi-Fi interfaces cannot be removed without damaging or destroying the device.

This project intends to utilize a passive receiver—perhaps even a set of reprogrammed IoT devices—to listen to a different, heavily populated IoT network. By watching patterns, we can correlate back to a specific device, even in a cacophony of traffic.



## Realizing the Power of Near-Term Quantum Technologies

191313 | Year 1 of 2 | Principal Investigator: J. E. Moussa

### Project Purpose:

Within 5-10 years, quantum information R&D is expected to yield “pathfinder” devices that demonstrate the promise of quantum technologies for national security problems. These near-term quantum devices will be able to create, maintain, and control quantum coherence with high fidelity. However, they will not be sufficiently mature for full-scale quantum computation because they will be incapable of quantum error correction and nontrivial algorithms simultaneously. It is believed that such devices can still be utilized for special-purpose computational tasks, such as materials simulation and optimization and quantum sensors—applications that will help further mature the technology. These quantum devices will need a support infrastructure of classical computers and software; the quantum device will, in effect, be a “quantum coprocessor” to a classical computer.

We propose to develop two key components of a quantum device support infrastructure that are targeted at analog quantum simulators, but sufficiently general purpose to be broadly applicable. The first is parameter-space compression, which will identify properties of quantum devices that are robust to noise, which sets limits on the computational power of a noisy quantum device. The second component is maximum-entropy reconstruction, which will estimate the values of hidden properties from properties that can be measured. This will enable additional computational power from a quantum device when direct measurements are limited.

The proposed infrastructure will be applied to quantum devices developed at Sandia in the coming years. Our approach of tight integration between quantum devices and classical software is a strategic route to near-term quantum supremacy.

The proposed research—to design algorithms that derive computational benefit from small, imperfect “quantum coprocessors”—is a novel and mostly unexplored direction. Small-scale theoretical assessments should precede and guide future experiments.

This project will build quantum capabilities at Sandia in next-generation hardware and software to complement its strong existing classical capabilities, helping to bridge the gap and open new possibilities for quantum technologies for national security.

## Reconfigurable Structure Coupler for Antenna Mode Excitation

180861 | Year 2 of 3 | Principal Investigator: N. J. Smith

### Project Purpose:

Robust antenna solutions are critical for modern sensing, tagging, tracking, and locating, RADAR, and other wireless systems. Antenna miniaturization has been a recent research topic as communication systems continue to become more mobile. While good progress has been achieved, antennas remain large and bulky, especially at low frequencies where they are naturally tens of feet or larger. For field applications, it is not feasible to erect an antenna of such size. Current antenna miniaturization techniques sacrifice efficiency and gain to reduce physical size. System link margins drive antenna gain specifications, setting the antenna’s size. To mitigate this problem, along with the issue of portability for large antennas, we propose a solution that will turn an existing metallic object into a radiating antenna. This is accomplished by developing an antenna mode excitation coupler (AMEC) that would attach to an existing metal object (fence, file cabinet, electrical wiring, etc.) to create the required current distribution facilitating radio frequency radiation. In many cases, a mobile antenna is no longer required; rather, existing metal structures are excited with a portable AMEC system. Research will include defining the required conditions to make a continuous metallic structure radiate, bounding the impedance matching range, properly coupling the AMEC to the structure, and development of reconfigurable phase shifters and matching networks accommodating different sized structures and operating frequencies. This work will be highly synergistic with reconfigurable antennas and array R&D at Sandia. If feasible, the AMEC concept will revolutionize a wide range of wireless applications.



## Rocket Engine Test System for Development of Novel Propulsion Technologies

176311 | Year 3 of 3 | Principal Investigator: W. Saul

### Project Purpose:

A novel small-scale rocket engine testing capability is needed for development of new propulsion systems—specifically “green” propellants that eliminate toxicity of current systems. By leveraging Sandia’s unique background in propulsion systems engineering with cutting-edge instrumentation and imaging techniques being developed at New Mexico Institute of Mining and Technology (NMT), the result will be a testbed for propulsion initiatives developed at both institutions.

To this end, A 150 lb<sub>f</sub> thrust class, modular, bi-propellant, rocket engine/gas-generator and supporting test infrastructure has been developed in a cooperative effort between Sandia and the NMT’s Energetic Materials Research and Testing Center. This modular test engine design consists of a head end fuel-oxidizer injector, a spark ignition gaseous H<sub>2</sub>/O<sub>2</sub> torch igniter, combustion chamber, and nozzle module. This robust design allows for rapid configuration changes as well as economical repair should hardware become damaged in testing. The engine interfaces with a permanently installed pressurizing system capable of delivering liquid nitrous oxide and a variety of liquid fuels for both rocket engine development and propellant performance evaluation. The regulated high pressure systems allow for delivery of liquefied gases above their saturation pressure as well as allowing for high pressure rocket engine/gas-generator operation. The facility test cell houses a 1 ton thrust capacity test stand leaving room for larger scale engine development.

Initial testing of the modular bi-propellant rocket engine involved evaluation of nitrous oxide and ethanol as potential “green” rocket propellants. Thrust and pressure measurements along with high-speed digital imaging of the rocket engine exhaust plume were conducted. Prompt starting without pressure oscillation or instability was demonstrated. Nitrous oxide and ethanol were shown to perform well as rocket propellants, with specific impulses experimentally measured in the range of 250 to 265 lb<sub>f</sub>-sec/lb<sub>m</sub> at ground level operating conditions.

## Simulation of Optical Phenomena in the Upper Atmosphere

173491 | Year 3 of 3 | Principal Investigator: W. C. Sailor

### Project Purpose:

The purpose of this collaborative project with Rensselaer Polytechnic Institute was to discover the appropriate theory to the simulation of optical phenomena (aurora) in the upper atmosphere and identify the governing equation. We wanted to investigate how the upper atmosphere responds to a large scale energetic disturbance. Previous approaches used assumptions that are not always valid, as well as unorthodox numerical methods. This project was a first-principles approach that avoided these pitfalls. This required understanding quantum theory, transport theory, atmospheric physics, integro-differential equation theory, complex variable theory, and numerical theory.

The governing equation for electron transport was derived from first principles (electron transport is the main catalyst to any aurora). A robust numerical method for solving the transport equation was developed that avoided unrealistic assumptions. Further, the method is well grounded in the field of numerical analysis. A basic theoretical model for auroral light emissions was developed that could yield these emissions as a function of altitude, latitude, and longitude. The emissions model contained both the effects of the electron transport and the naturally occurring dynamics of the upper atmosphere.

Auroral research helps us better understand the response of our atmosphere to a large scale energetic disturbance, in addition to the coupling between the various parts of the atmosphere (i.e., thermosphere, ionosphere, magnetosphere, etc.). Further, the strength of an aurora is correlated to the strength of solar activity and may provide a measure of radiation on space assets.



## Social-Media Account Resolution and Verification

190990 | Year 1 of 2 | Principal Investigator: D. Garcia

### Project Purpose:

The purpose of this project is to develop algorithms that can detect identity deception on social networks by augmenting natural language analysis with graph, temporal, and metadata features. On social media platforms, users are generally allowed to create any account they choose and enter “personal” information that is rarely verified. Hence social media accounts are often used for illegal purposes, including identity theft, money laundering, terrorist and insurgent activities, cyber attacks, etc. Social media is the perfect place for people with illegal purposes to meet, recruit, and coordinate, as it provides anonymity and cyber crimes are rarely prosecuted.

Current work in identifying deceptive actors focuses principally on text analysis and rarely takes advantage of other aspects of that account’s activity such as temporal patterns or social graphs. Author attribution analysis has been done multiple times, mostly on large works such as books. There is little work being done on attempting attribution of small, dynamic content such as tweets or posts.

We will develop algorithms to identify accounts being used for nefarious purposes and aid in determining authorship of the account. We believe that combining post content, social and interaction graphs, and temporal activity into one analysis, we can find deceptive users that would be missed by any one-feature analysis. These techniques will allow us to identify multiple accounts authored by the same person (one-to-many) as well as single accounts authored by multiple actors (many-to-one). These techniques will be developed and tested with publicly

## Staghorn: An Automated Large-Scale Distributed System Analysis Platform

180824 | Year 2 of 2 | Principal Investigator: K. G. Gabert

### Project Purpose:

Sandia has developed large-scale emulation-based cyber analysis platforms (e.g., Firewheel). This project builds on the significant investment Sandia has made in Firewheel by creating a new analysis platform for large-scale distributed systems: Staghorn. This platform is based on a novel primitive—the ability to take a snapshot of the entire distributed system that includes both its network and input/output state. This primitive opens up the possibility for many avenues of analysis, ranging from “single stepping” through a massive system’s execution, to forking execution at a given point in time, in order to vary system inputs and find optimal configurations.

There are numerous technical challenges in constructing such a system, including significant modifications to key Linux virtualization and networking components and development of an algorithm to perform distributed snapshots that include network state. Each challenge has been shown possible through our own experience in developing Firewheel and recent academic publications. Staghorn’s contribution is to tie each challenge together to form the first large-scale emulation-based distributed system analysis platform.

Staghorn opens the door to a host of new analyses for emulation-based models containing numerous virtual machines. It enables researchers to discover, study, and fix bugs in large distributed applications; it provides significant improvements in debugging; it supports understanding and measuring nondeterminism within specific parts of a model; it can be used to take advantage of common execution prefixes; and it can be leveraged within training environments to contain participant mistakes.



## Trusted Materials using Orthogonal Testing

180857 | Year 2 of 3 | Principal Investigator: M. Van Benthem

### Project Purpose:

The purpose of this project is to prove (or disprove) that a reasonable number of simple tests can be used to provide a unique data signature for materials, changes in which could serve as an indication of material deviation, prompting further evaluations. The routine tests are mutually orthogonal to any currently required materials specification tests.

Materials represent the building blocks for all physical products. Unanticipated materials changes can result in undesirable and costly consequences in product reliability and performance. These changes may result from a vendor's process improvements driven by technological advances and/or economic considerations. Of greater concern is the manufacturer's, and in turn the consumer's, vulnerability to potential nefarious actions. The functional impact of integrating dubious materials into the manufacturing process spans the range from processing and fabrication through reliability assessment activities, as anomalies may manifest early or be aging-related.

One method of addressing the materials assurance process is to use an array of material specifications. Functionally, these specifications may range from weak (manufacturer part number) to robust (a comprehensive series of physical or chemical tests). However, the potential for detrimental material changes going undetected while using the existing specifications dictates that we develop a new testing paradigm to verify that materials are precisely those that are required for their intended purpose. We have proposed a new approach for assuring materials, complementing the current specifications process. The orthogonal testing (OT) approach could be a complete paradigm shift for how we accept incoming materials and fabricated parts. In this new paradigm, we would only use OT during refurbishment to determine that the material is, or is not, from the same family that was qualified.

## Using Linkographies of Cyber Attack Patterns to Inform Honeypot Placement

173035 | Year 3 of 3 | Principal Investigator: J. C. Jarocki

### Project Purpose:

Several research and development projects have deployed honeypots, honeynets, and honeytokens to confuse, slow, and detect cyber adversaries. However, the placement of these resources is typically agnostic of the behavior patterns and goals of the adversaries. This project focuses on learning adversarial patterns during cyber attacks so that the placement of false flags can be chosen to minimize attacker goals while maximizing defensive objectives.

To explore this space, we propose applying research from a different domain: shopping behavior and store layout. El-Khouly and Penn have constructed models of human behavior in stores such as Ikea that demonstrate how shopper flow can be consistently guided along a path that causes minor frustration while leading to unintended purchasing choices. This series of steps along the path can be represented as a linkograph: a directed path through an undirected graph of events over time. By acquiring data on cyber attack steps from real incidents, we can construct similar representations for normal patterns of adversarial understanding, behavior, and activity through a target network. Armed with this information, defenders can reduce the intelligibility of the target network and maximize the effort an adversary must apply to complete the mission.

This project explores new methods to gain insight into cyber attacker behavior and response to stimuli, seeding future research with data and methods for modeling attacker interactions. This work involves arraying defenses and decoys in real time on a live network using experimental models—a technology area that is presently underdeveloped.





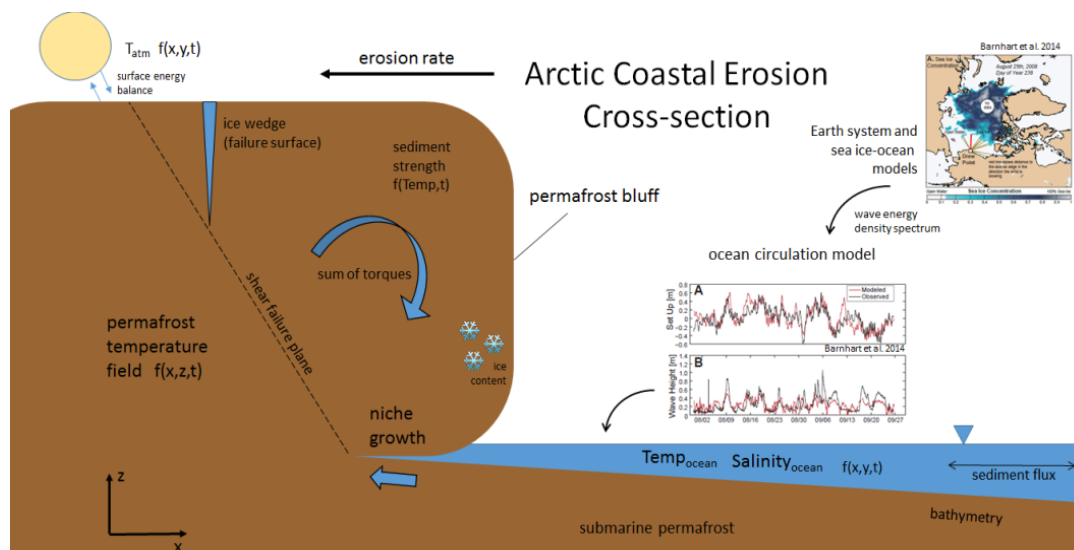
## Using Machine Learning in Adversarial Environments

173037 | Year 3 of 3 | Principal Investigator: W. L. Davis, IV

### Project Purpose:

Intrusion/anomaly detection systems are among the first lines of cyber defense. Commonly, they either use signatures or machine learning (ML) to identify threats, but fail to account for sophisticated attackers trying to circumvent them. We propose to embed machine learning within a game theoretic framework that performs adversarial modeling, develops methods for optimizing operational response based on ML, and integrates the resulting optimization codebase into the existing ML infrastructure developed previously. Our approach addresses three key shortcomings of ML in adversarial settings: 1) resulting classifiers are typically deterministic and, therefore, easy to reverse engineer; 2) ML approaches only address the prediction problem, but do not prescribe how one should operationalize predictions, nor account for operational costs and constraints; and 3) ML approaches do not model attackers' response and can be circumvented by sophisticated adversaries. The principal novelty of our approach is to construct an optimization framework that blends ML, operational considerations, and a model predicting attackers reaction, with the goal of computing optimal moving target defense. One important challenge is to construct a realistic model of an adversary that is tractable, yet realistic. We aim to advance the science of attacker modeling by considering game theoretic methods and by engaging experimental subjects with red teaming experience in trying to actively circumvent an intrusion detection system, and learning a predictive model of such circumvention activities. In addition, we will generate metrics to test that a particular model of an adversary is consistent with available data.

Little research has been conducted to date on providing a mathematical framework for rigorously analyzing the impact of defensive postures (e.g., network configurations) on the interactions between cyber defenders and adversaries. This work is novel and risky; yet, if successful, could serve as the catalyst for extending theoretical understanding of interactions towards practical decisions that will improve computer security.



## Energy and Climate

The Energy and Climate (EC) IA is focused on research and development that advances the state of knowledge and overcomes barriers to deployment of energy technologies for both supply and demand. The investment area seeks R&D that leverages Sandia's differentiating capabilities to create opportunities that can be transformational relative to current technologies or approaches, and encourages building directly on the results of fundamental research to provide real solutions to the most pressing mission challenges. The EC IA promotes research and development that supports the goals of the Secure and Sustainable Energy Future (SSEF) and related Mission Areas (MAs). The SSEF MA seeks to make national-level differentiating contributions to the nation's energy security and resilience, economic viability, and environmental sustainability. To achieve this vision, the MA targets SNL's strengths toward areas of greatest potential impact within three main strategy elements: Stationary Power, Climate and Earth Systems, and Transportation Energy.

*The image above shows a conceptual illustration of the block erosion process, including the physics believed necessary to accurately predict erosion. This project investigated innovative methods to unite wave and circulation patterns and coastal erosion to assess the impacts of Arctic change on existing and future infrastructure. (Project 198982, Integration of Climate and Wave Models to Evaluate Arctic Erosion Caused by Melting Sea Ice)*

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## A Fundamental Study on the Physicochemical Process of Soot Particle Inception

191017 | Year 1 of 3 | Principal Investigator: S. A. Skeen

### Project Purpose:

This project attempts to identify the large hydrocarbons (macromolecules) associated with incipient soot in combustion environments at low, moderate, and high (i.e., engine-relevant) pressures. The goal is to provide kinetic mechanism developers with fundamental knowledge leading to an accurate representation of soot inception in models used for the design and optimization of next generation engines. Prior efforts to identify incipient soot's chemical composition with mass spectrometry have been limited by probe perturbation, poor spatial and temporal resolution, insufficient sensitivity, and the overwhelming number of species observed in the soot-forming regions. Detailed chemical information has also been unattainable by nonperturbative spectroscopic techniques, which are hampered by the broad and overlapping absorption spectra of large hydrocarbon molecules.

Novel flame, pyrolyzing-spray, and combustor-spray sampling techniques are under development that will allow us to exploit the atomic-level sensitivity of surface science diagnostics toward the characterization of macromolecules and soot nuclei deposited on substrates. We have acquired some reference data for potential soot nuclei components using various state-of-the-art microscopies. We intend to measure dimer binding energies to evaluate their propensity for nucleation and investigate physicochemical changes occurring after exposure to intermediate growth species. These data will support the characterization of flame-extracted samples, for which large candidate species and/or dimers have been isolated using a mass filter. Finally, we will determine the effects of pressure using a modified high-pressure spray vessel. Identification of the species associated with soot nucleation will provide the fundamental information necessary for later development of predictive engine models.

Identification of species associated with the nucleation of incipient soot has eluded researchers for 50 years. Sandia is uniquely positioned and has assembled a multidisciplinary team of combustion and materials scientists with the expertise and diagnostic tools necessary to approach the problem in a novel way.

## Advanced Fuel-Injection System for Rapid Control of High-Efficiency Low-Temperature Combustion Engines using Gasoline and other Gasoline-Like Fuels, Including Biofuels

180862 | Year 2 of 3 | Principal Investigator: J. E. Dec

### Project Purpose:

Establishing a secure energy future and mitigating carbon dioxide emissions requires significant improvements to the fuel efficiency of the nation's vehicle fleet. By far, the largest gains can be made by raising the efficiency of gasoline engines, which consume the majority of fuel and have much lower thermal efficiencies than diesel engines. Engines using low-temperature gasoline combustion (LTGC) can provide efficiencies above those of diesels, improving fuel economy by 30 to 40% over current gasoline engines. A key impediment to the commercialization of LTGC is that current techniques for controlling ignition timing over the load-speed map are complex, insufficiently robust, and have difficulty with rapid transients. This project would develop and demonstrate an advanced fuel-injection system to provide the required robust, rapid control. Leveraging Sandia's expertise in microfluidics and LTGC engines, this fuel-injection system would precisely adjust the combustion timing on an injection-by-injection basis as the engine traverses the operating map. Despite the risks, this project is based on sound fundamentals, and this technology could be a "game changer" for the commercialization of LTGC engines, with benefits for energy security and the environment.



## Aggregating Distributed Energy Resources as Secure Virtual Power Plants

180867 | Year 2 of 3 | Principal Investigator: J. Johnson

### Project Purpose:

The goal of the project is to create optimization and control tools to increase the quantity of variable, nondispatchable renewable energy on electric distribution systems by providing electric utilities with a greater capacity to perform voltage/frequency regulation and respond to grid disturbances. This capability has been established through virtual power plant (VPP) software consisting of a cyber-resilient, real-time communications system that connects to multiple heterogeneous distributed energy resources (DERs). The VPP optimizes the behavior of distributed power electronics-based converters to provide services traditionally reserved for larger power plants (e.g., spinning reserve, inertial damping, and voltage/ frequency regulation). The individual DERs are scheduled with a day-ahead economics-based stochastic optimization tool that incorporates renewable energy power forecasts and a centralized, cascading control system that issues commanded advanced grid functions to provide ancillary services via real and reactive power flows to the grid. However, the VPP construct necessitates communications to distribution-level devices at residential and commercial facilities over wired and wireless Internet channels. The inherent unsecure nature of these communications increases the risk of an adversary potentially leveraging a VPP to control large quantities of grid-connected generators, ignore or spoof supervisory control and data acquisition (SCADA) signals, manipulate bids on energy exchanges, or instigate grid instabilities. Therefore, this project has established a novel, broadly applicable VPP security posture that includes: 1) intelligent enclaving strategies to isolate DER resource pools from single point incursions, 2) intrusion detection systems, and 3) dynamic reallocation of DER operations based on communication failures and natural/adversarial attacks. This R&D effort has far-reaching implications in electric grid distribution level controls, forecasting, and cybersecurity. The cyber-secure communications and resilient controls will be demonstrated at Sandia's Distributed Energy Technologies Laboratory (DETL) by aggregating renewable and traditional distributed energy resources.

## An Advanced Decision Framework for Power Grid Resiliency

173090 | Year 3 of 3 | Principal Investigator: J. Watson

### Project Purpose:

The national power grid is the foundational infrastructure upon which our economy, national defense, health care, emergency response, and standard of living rely. Grid resiliency is, therefore, imperative — grid control systems must prepare for and adapt to changing conditions and withstand and recover rapidly from disruptions, whether caused by accidents, naturally occurring threats, or deliberate attacks. Two key factors drive our need to boost grid resilience: the increasing frequency and magnitude of natural disasters, and tighter linkages with other infrastructures (e.g., cyber) driven by grid modernization efforts.

Current performance metrics for power systems address reliability, but they neither quantify resiliency nor consider delivery failure consequences. Without guidance from rigorous metrics, grid operators are ill prepared to anticipate and operate through large-scale cascading failures and blackouts, and lack analytical capabilities to support restoration. We propose to develop foundational grid resiliency metrics and leverage state-of-the-art simulation and decision analysis tools to devise a novel control system to support operate-through and restoration.

The project will implement an advanced anticipatory decision architecture that will guide the system in order to maximize expected future resiliency. System inputs include a description of the grid control elements and the range of their feasible values in each of many projected scenario trajectories. We will employ stochastic and robust optimization paradigms as the core decision formalism in our proposed framework. Sandia's Pyomo optimization system will be leveraged and extended to express and solve the resulting nonlinear anticipatory decision problems.

The project is developing core metrics and technologies required for resilient grid infrastructures. Resiliency metric development is a complex, iterative process involving multiple stakeholders with disparate interests. Metric acceptance is key and requires social, institutional, and technical analyses. The proposed grid control system requires integration of state-of-the-art analytic techniques, including uncertainty quantification, predictive simulation, optimization, and high performance computing.





## Co-optimization to Integrate Power System Reliability Decisions with Resiliency Decisions

191057 | Year 1 of 3 | Principal Investigator: B. J. Pierre

### Project Purpose:

This project is developing algorithms and general-purpose software tools important to co-optimization of electrical system infrastructure improvements to simultaneously enhance both reliability and resiliency. Such co-optimization is not presently performed. Upon completion, this project will provide tools that could potentially:

- Inform stakeholders of cost effective infrastructure investment decisions that simultaneously improve both reliability and resilience
- Inhibit impacts to resilience at the expense of reliability or vice versa
- Characterize tradeoffs between resiliency and reliability, for given infrastructure investment decisions
- Quantify both reliability and resilience impacts of proposed investments

The topic of resilience and reliability of the US electric infrastructure fits within the goals of DOE and Sandia's national security missions.

The project will provide unique and differentiating value to the energy sector by identifying investments that beneficially impact both reliability and resiliency. The computational challenge of the proposed co-optimization effort is significant, such that industry will not fund the basic research required for development and eventual deployment.

## Development of Detection and Mitigation Algorithms for False Data Injection Cyberattacks against Nuclear Facilities

193419 | Year 1 of 3 | Principal Investigator: K. Groth

### Project Purpose:

Cybersecurity is a serious ongoing challenge that can impact national security, public safety, and the national economy. Signal tampering is a significant threat with serious consequence for the energy sector, including coordinated energy blackouts and initiation of accidents by malicious and nonmalicious adversaries. The possibility of a false data injection (FDI) attack has been recently recognized by cybersecurity experts as a significant threat with serious consequences. In an FDI attack, adversaries may manipulate the readings of multiple sensors and control systems. The most serious FDI attacks involve attackers, informed by subject experts, injecting data which falls into the normal range of the sensor readings. This defeats conventional state estimation algorithms and allows attackers to avoid detection. Detecting these FDI attacks is of critical importance to the safe operation of nuclear power and other energy infrastructure.

This project aims to develop a suite of real-time computational algorithms capable of distinguishing between FDI attacks and normal sensor readings (e.g., variations due to normal operational changes), with a specific demonstration to the flux state estimation problem inside a nuclear reactor core. To achieve this goal, the proposed algorithms will provide quantitative understanding of the uncertainty sources that are responsible for the observed deviations between sensor measurements and simulation results. This understanding is critical to detecting serious FDI attacks, wherein signals are otherwise indistinguishable from normal deviations found in plant signals.

This is a collaborative effort with Purdue University.



## Dynamic Simulation and Optimization of Resilient Hybrid Microgrid Systems

193766 | Year 1 of 1 | Principal Investigator: R. Guttromson

### Project Purpose:

The overarching purpose of this project, in partnership with the University of Illinois, is to produce a simplified top-level technical model integrating hybrid energy production into microgrids as a preliminary test case for potential later scale-up, first to regional and later to the national electric grid. This work creates, then optimizes, models of complex dynamic hybrid microgrid systems involving multiple energy technologies.

A microgrid is essentially a complex system that can have multiple energy generation sources serving users, with increased overall reliability produced through diversity in an energy generation portfolio. Integrating the users is relatively simple—but integrating the sources to provide reliable power with finite funding is exceptionally difficult. And what are the benefits of resiliency versus the costs to integrate a diverse complement of renewable sources into a microgrid? The problem is answered at a top level by modeling technical and financial barriers to integration while generating top-level metrics regarding grid resiliency. Development of this model provides capability to quantify possible future integration of novel and low technology readiness level energy sources into the microgrid early in development to help guide energy developer stakeholders. Through this modeling, insight is generated into the relative sensitivity of complex intertwining factors such as technology integration, taxation policies, and regulation.

Energy technologies that will be considered include nuclear, coal, and natural gas for primary generation; wind, solar-thermal, and solar-photovoltaic for renewable generation; electrical, thermal, mechanical, and chemical storage; and energy resources such as a chemical plant to convert thermal and electrical power into fuels.

## Electrostatic Coating with Naked Copper Nanoparticles

173495 | Year 3 of 3 | Principal Investigator: T. J. Boyle

### Project Purpose:

In collaboration with the University of Arizona, low-cost nanoinks for interconnect applications will be developed, focusing on nanocopper inks. An alternative coating method that allows for conductive film formation on a variety of substrates is desirable, both as an alternative to conventional conductive thin-film processing as well as the emerging field of flexible electronic and photovoltaic devices. In conventional approaches, a metal catalyst is used that can be both expensive and increases the resistance of interconnect lines. An alternative approach to the formation of copper thin films is electroless deposition (ELD). The ELD process applies the use of colloid suspensions of metallic nanoparticles (NP) attracted to a substrate surface and allows for a number of bottom-up tailoring options to conductive pathway formation. NPs offer feature resolution that is dependent on controllable physical properties, and their electrochemistry may be tailored to eliminate grain growth catalysts. The use of NPs over a bulk phase allows for the bottom-up creation of electric paths that conform to the local shifts in position of the underlying layer and are formed at moderate (<673K) temperature. ELD films may conduct current in low thermal budget applications, where the substrate undergoes macroscopic flexing. Metallic NP films are integral to low-cost electrically-conductive applications such as flexible electronics, RFID tags, antennas, and power distribution applications.



## Foundations for Protecting Renewable-Rich Distribution Systems

191059 | Year 1 of 1 | Principal Investigator: A. Ellis

### Project Purpose:

High proliferation of inverter interfaced distributed energy resources (IIDERs) into the electric distribution grid introduces new challenges to protection of such systems. This is because the existing protection systems are designed with two assumptions: 1) system is single-sourced, resulting in unidirectional fault current and 2) fault currents are easily detectable due to much higher magnitudes compared to load currents. Due to the fact that most renewables interface with the grid through inverters, and inverters restrict their current output to levels close to the full load currents, both these assumptions are no longer valid—the system becomes multi-sourced and overcurrent-based protection does not work.

The primary scope of this study is to analyze the response of a grid-tied inverter to different types of faults in the grid and investigate methods for detection of faults at output of the inverter. We will develop high-fidelity models for an inverter and IEEE 13-node distribution grid. Different types of faults and capacitor switching events are simulated at various locations, and variations in inverter output currents and voltages are observed. Based on the observations of these waveforms, three strategies are examined to reliably detect fault:

- Quantifying and using the transient content in the inverter output: a sophisticated time-frequency resolution technique is used for fast quantification of the transient content of voltage and current generated by the inverter
- Using zero-sequence current magnitude at the high side of the interfacing transformer: though inverter produces only positive sequence currents even for unbalanced faults, the transformer secondary helps detect ground faults due to its contribution to zero sequence currents to ground faults
- Using voltage drop at the transformer terminals: although inverter currents are limited, the grid faults still result in lowering of system voltage. This is also considered an indicator of fault.

## Fractal-Like Materials Design with Optimized Radiative Properties for High-Efficiency Solar Energy Conversion

173092 | Year 3 of 3 | Principal Investigator: C. K. Ho

### Project Purpose:

High temperature solar receivers and radiative heat collection components are used in renewable energy systems, space and satellite applications, and military operations. The purpose of these components is to collect heat by maximizing solar absorption while minimizing thermal losses. However, at high temperatures (receivers can reach 600 °C and higher), the radiative losses are significant. While previous studies have tried to improve the efficiency of these receivers at high temperatures by increasing solar absorptivity and reducing thermal emissivity of surface coatings, very little research has investigated the optimization of features and radiative properties of receivers and other components at multiple length scales. Our project will develop fractal-like structures and designs at multiple scales (millimeters to meters) that will maximize solar absorption while minimizing heat loss. Through our background research on radiative properties of surfaces, we have identified that self-similar features of fractal structures over a large topological dimensional range will provide an effective trapping mechanism for solar irradiation. In addition, synthesis and design of fractal-like structures will be tailored to reduce reflective losses, local view factors, and thermal emittance at multiple scales. Novel radial and star-like patterns recently introduced at the macroscale have been shown to reduce radiative view factors by up to 70% and total heat loss by 50%. Incorporation of these hierarchical features and designs at multiple scales are expected to significantly increase thermal efficiencies of solar energy receivers and a broad range of thermal collection devices for sustainable, lower-cost, high-efficiency energy conversion.

The project aims to develop novel designs for high temperature solar thermal receivers with increased efficiencies that address DOE's mission to develop sustainable energy technologies. The work requires complex modeling, as well as testing available only at Sandia's National Solar Thermal Test Facility, that will answer fundamental radiative transfer questions to improve the performance of solar thermal receivers.



## Fundamental Properties of Confined Enzymes

195702 | Year 1 of 1 | Principal Investigator: S. Rempe

### Project Purpose:

In his 2015 State of the Union Address, President Obama said, “no challenge poses a greater threat to future generations than climate change.” Governments worldwide have pledged to combat climate change by reducing carbon dioxide (CO<sub>2</sub>) emissions from the power sector. Power plants that use coal and natural gas to generate electricity currently account for nearly half of the 40 billion tons/yr of CO<sub>2</sub> emitted by human activities worldwide. Domestic and global CO<sub>2</sub> emissions are widely expected to increase over the next quarter century despite investments in renewable and low-carbon fuels for electricity. The increasing global demand for cheap, dependable electricity to support economic well-being drives fossil fuel-based power and the consequent carbon pollution. The US has called for 30% reduction in CO<sub>2</sub> emissions for new and existing power plants. Lack of an efficient CO<sub>2</sub> separation technology hinders compliance. Current technology is prohibitively costly, almost doubling the cost of electricity generated. Those flaws threaten access to cheap, dependable electricity. A transformational CO<sub>2</sub>-separation technology is critically needed.

Sandia’s recent advances in an ultra-thin liquid membrane for gas separation provide a potential environmentally friendly solution for cost-effective CO<sub>2</sub> separation. To help realize this potential, a molecular-level understanding is needed to permit optimization of this unique membrane’s design. The membrane active layer consists of nanopores that trap a thin (~20 nm) layer of water loaded with enzymes that selectively catalyze CO<sub>2</sub> uptake and release. The sensitive CO<sub>2</sub> flux depends on nanopore surface chemistry in the active region. To understand that dependence, we applied molecular simulations to interrogate enzyme behavior in the presence of varied surface chemistries.

## Fundamentals of Pellet-Clad Debonding

191056 | Year 1 of 3 | Principal Investigator: R. P. Dingreville

### Project Purpose:

This project provides a fundamental understanding of the complex mechanisms of interfacial damage and aging processes associated with pellet-clad debonding (PCD) considering environmental and microstructural factors. This will be accomplished using a unique suite of in situ nanoscale experiments on surrogate interfaces integrated with a multi-resolution computational framework and calibrated with decommissioned commercial spent fuel.

This project systematically investigates degradation mechanisms contributing to PCD by:

- Experimentally characterizing, in detail, the impact of microstructural features (interface roughness, grain size, texture) and environmental factors (thermal/irradiation) on the mechanical properties changes of pellet/clad interfaces
- Developing calibrated predictive models using the acquired experimental results to simulate complex interfacial systems (surrogate and spent nuclear fuel [SNF]) over a broad range of environmental conditions.



## High-Resolution Modeling and Measurements in the Arctic

191055 | Year 1 of 3 | Principal Investigator: E. L. Roesler

### Project Purpose:

Diminishing sea ice in the Arctic causes more exposed ocean to uptake solar radiation, setting up a positive feedback that leads to further melting. Low clouds have been identified as potentially increasing sea ice melt by warming the surface below them. The relationship between sea ice and low clouds cannot be proved with global climate models (GCMs) because they are erroneous in calculating clouds in the Arctic. The purpose of this project is to investigate our hypothesized source of this error, the low resolution of GCMs, and improve our understanding of Arctic low clouds. The technical challenge will be to develop a variable resolution GCM with an embedded high resolution model in every column to resolve vertical motion. Once this model is developed, we will verify it by comparing with high-resolution vertical measurements taken with liquid water sensors on a tethered balloon. We plan to also use ground-based and space-based radiometric measurements to compare with the tethered balloon measurements. In each step of our model development, we plan to compare the new result with the low resolution GCM and to the observations. This research is notably different for two key reasons. First, a variable resolution GCM with an embedded high resolution model has never before been developed. Second, in situ cloud data collected from a tethered balloon has never before been compared to an variable resolution GCM or other high resolution model. By combining measurements and models, we anticipate an improved understanding of Arctic low clouds and their relationship to sea ice.

## Holographic Spectrum Splitting Demonstration System for Dual Photovoltaic and Biofuel Operation

180870 | Year 2 of 2 | Principal Investigator: W. C. Sweatt

### Project Purpose:

The overall aim of this research is to create spectrum splitting optical elements that enable increased conversion efficiency and energy yield in a photovoltaic (PV) module. Lateral spectrum splitting is an optical technique for multiple-bandgap PV module design. Bandgaps are placed side-by-side while a dispersive optical element redistributes the spectrum across the cells. A spectrum splitting module does not require lattice matching, so PV bandgaps can include a greater range of materials. The lateral arrangement may also allow swapping-out PV cells during the course of the module's lifetime. This would allow flexibility of the module to update PV cells or to repair individual components of the module. Additionally, like-bandgaps can be connected to separate inverters to eliminate current-matching constraints, increasing power output under a varying solar spectrum. The challenge of spectrum splitting lies in cost, complexity, and manufacturability.

In this project, two types of diffractive optical elements (DOEs) are explored in their application to photovoltaic spectrum splitting: a freeform surface relief DOE and an off-axis volume holographic lens. The design process for each optic is thoroughly investigated with key design parameters highlighted. Measured performance of each DOE is also included. Performance is analyzed with spectrum splitting metrics developed in our research group. Simulation of the DOEs is also performed. For the holographic lens, a full system model is incorporated into modeling software to evaluate power output and annual energy yield. The advantages and disadvantages of each DOE is studied. Overall, both designs have comparable performance with sharp spectral filtering and >80% optical efficiency in the desired spectral bands. If further steps are taken to control the fabrication process, these optical components will approach their theoretical performance.





## Integration of Climate and Wave Models to Evaluate Arctic Erosion Caused by Melting Sea Ice

198982 | Year 1 of 1 | Principal Investigator: J. D. Roberts

### Project Purpose:

This project identifies the unique, critical, and rapidly growing challenge posed by Arctic coastal erosion and outlines innovative solutions to significantly improve Arctic coastal erosion predictions to potentially inform hazard/risk assessment and response planning.

Permafrost-dominated coastlines in the Arctic are rapidly disappearing. Arctic coastal erosion rates in the US have doubled since the middle of the twentieth century and appear to be accelerating. The American and Canadian coastlines exhibit the highest erosion rates in the Arctic, as high as 22.5 m/yr. Positive erosion trends have been observed for highly variable geomorphic conditions across the entire Arctic, suggesting a major (human timescale) shift in coastal landscape evolution. Unfortunately, irreversible coastal land loss in this region poses a threat to native, industrial, scientific, and military communities.

It is now thought that rapid alterations to the Arctic coastline are facilitated by oceanographic and geomorphic perturbations associated with climate change. Sea ice extent is declining, sea level is rising, sea water temperature is increasing, and the permafrost thermal state is changing. The polar orientation of the Arctic exacerbates the magnitude and rate of the environmental forcings that facilitate coastal land area loss. While the fundamental mechanics of these processes are understood, their nonlinear combination is understudied and poses an extreme hazard. Tools to accurately predict Arctic coastal erosion do not exist. To obtain an accurate predictive model, a coupling of the influences of evolving wave dynamics, thermodynamics, and sediment dynamics must be developed. This project outlines the key first step towards creating a coupled model for the quantification of coastal hazards that will allow for sustainable planning and development of Arctic infrastructure.

## Investigating the Chemistry, Physics, Wear and Aging in Rolling Electrical Contact

191053 | Year 1 of 3 | Principal Investigator: W. L. Staats, Jr.

### Project Purpose:

As of 2016, a practical approach to the longstanding question of carbon-free renewable energy is beginning to emerge. It now appears that a combination of wind, solar-photovoltaic power, and battery-based grid storage has genuine potential to become economically viable without subsidies. Recent breakthroughs in cost-effective aqueous flow battery technology is one of the most notable recent developments. But in the area of wind, the question of scalability has yet to be resolved. Wind turbine manufactures worldwide are now switching from gearbox-plus- induction-generator drive trains to permanent magnet direct drive generators to meet requirements for reliability. But such direct drive wind turbines require massive quantities of rare earth materials (neodymium, dysprosium) for fabrication of the permanent magnets used in generator rotors. The amount of rare earth materials that will be required to construct the wind portion of our renewable energy economy is completely prohibitive. Mining of rare earths is also highly damaging to the environment. The Twistact technology utilizes a new type of rotary electrical contact that eliminates the need for rare earth magnets by substituting copper and steel (i.e., electromagnets). Because the Twistact functions in a previously unused parameter space, namely electro-tribo-chemistry of extended rolling electrical contact, there is no relevant scientific study nor practical experience. Our project addresses this interesting area of research and investigates the surface chemistry and physics that govern time and current density dependent phenomena in this regime. These studies will help in the understanding of fundamental aging and wear mechanisms.



## Lithium Oxysilicate Compounds as Stable Analogs for Understanding Li-P-S High Rate Li-Ion Separators: Moving Solid Electrolytes into High Rate Applications

181205 | Year 2 of 3 | Principal Investigator: C. A. Apblett

### Project Purpose:

The purpose of this project is to study an alternative to current solid state lithium ion ( $\text{Li}^+$ ) conducting solid electrolyte interphase (SEI) layers to improve the safety and reliability of lithium battery systems. Current lithium ion batteries suffer from low energy density in part due to the relatively low capacity of the negative (anode) terminal chemistry. Moving from the current carbon-based host to a silicon-based host for lithium would dramatically improve battery energy density, but the expansion of silicon on lithium insertion causes problems with the stability of the SEI on cycling. This SEI layer is formed organically from the decomposition of electrolyte on the silicon anode, but the fundamental understanding of the SEI is still very poor.

A new class of highly conductive  $\text{Li}^+$  solid phase conductors is being investigated based on lithium oxide-silicon oxide compounds, which have been studied little in the literature, but have an analog in the lithium oxynitride systems that have reasonable solid state mobilities. We will collaborate with University of Colorado-Boulder to support research into sol gel synthesis of these precursors as a model system. We will study the effects of composition and organic content on the nature, mechanical properties, and ion transport properties of this engineered SEI material. We will use both mechanical membrane-based measurements of stress in the films, as well as electrochemical measurements and control of stoichiometry in the sol phase to produce a model system that can be probed for its physical properties to gain some understanding into the nature of the silicon SEI in a real battery.

While the fundamental work in this project is far removed from building real power sources, the learning gained in understanding lithium transport in solid phases can help move forward safety and durability programs within Sandia for a range of power sources.

## Measurements and Modeling of Black Carbon Aerosols in the Arctic for Climate-Change Mitigation

173094 | Year 3 of 3 | Principal Investigator: H. A. Michelsen

### Project Purpose:

Growing evidence suggests that black carbon (BC) particles contribute significantly to global climate change and are largely responsible for the enhanced warming of the Arctic (~twice that of the global rate). Because of the relatively short atmospheric lifetimes of particulates compared to  $\text{CO}_2$  and the large radiative forcing of BC aerosols (23-65% that of  $\text{CO}_2$ ), BC reductions are being considered as a viable near-term climate change mitigation approach. Assessing the effectiveness of such a strategy, however, will require better estimates of BC climate forcing, which are hampered by large uncertainties associated with a paucity of atmospheric observational constraints, particularly in the Arctic, and poorly represented BC physical and optical properties in climate models. This project aims to reduce uncertainties on Arctic climate forcing of BC by combining Arctic field observations, advanced instrumentation and characterization, and climate modeling. In this project, we made continuous BC measurements in Barrow, Alaska semi-autonomously and combined laboratory experiments and modeling to characterize and improve commercial instrumentation used for BC field measurements. Additionally, we implemented a nudging approach to the Community Atmospheric Model (CAM) to test the physics that influences BC abundances in the Arctic. This project embodies a unique combination of Arctic field instrument deployment, which leverages Sandia's expertise in Arctic measurements; controlled laboratory experiments that exploit Sandia's unique capabilities in BC particle diagnostics; and climate modeling using the state-of-the-art Community Earth System Model (CESM). Although BC is measured using filter-based instrumentation in Barrow, our measurements are the first continuous measurements of BC in Barrow using a Single-Particle Soot Photometer (SP2). Our laboratory characterization of this instrument represents the first detailed modeling of the instrument behavior and provided unique and valuable information about instrument artifacts and possibilities for improvement. The use of the latest version of CESM capitalizes on the new Spectral Element Community Atmospheric Model (CAM5-SE) developed at Sandia.



## Meta Material Receivers for High Efficiency Concentrated Solar Energy Conversion

191058 | Year 1 of 1 | Principal Investigator: J. Yellowhair

### Project Purpose:

Operation of concentrated solar power receivers at higher temperatures ( $>700\text{ }^{\circ}\text{C}$ ) would enable supercritical carbon dioxide ( $\text{sCO}_2$ ) power cycles for improved power cycle efficiencies ( $>50\%$ ) and cost-effective solar thermal power. Unfortunately, radiative losses at higher temperatures in conventional receivers can negatively impact the system efficiency gains. One approach to improve receiver thermal efficiency is to utilize selective coatings that enhance absorption across the visible solar spectrum while minimizing emission in the infrared to reduce radiative losses. Existing coatings, however, tend to degrade rapidly at elevated temperatures. We will report on the initial designs and fabrication of spectrally selective metamaterial-based absorbers for high temperature, high-thermal flux environments important for solarized  $\text{sCO}_2$  power cycles. Metamaterials are structured media whose optical properties are determined by subwavelength structural features instead of bulk material properties, providing unique solutions by decoupling the optical absorption spectrum from thermal stability requirements. The key enabling innovative concept proposed is the use of structured surfaces with spectral responses that can be tailored to optimize the absorption and retention of solar energy for a given temperature range. In this initial study, in partnership with University of Texas at Austin, we use Tungsten for its stability in expected harsh environments, compatibility with microfabrication techniques, and required optical performance. Our goal is to tailor the optical properties for high (near unity) absorptivity across the majority of the solar spectrum and over a broad range of incidence angles, and at the same time achieve negligible absorptivity in the near infrared to optimize the energy absorbed and retained. To this goal, we apply the recently developed concept of plasmonic Brewster angle to suitably designed nanostructured Tungsten surfaces. We predict that this will improve the receiver thermal efficiencies by at least 10% over current solar receivers.

## Multi-objective Optimization of Solar-Driven, Hollow-Fiber Membrane Distillation Systems

180872 | Year 2 of 3 | Principal Investigator: T. M. Nenoff

### Project Purpose:

Securing additional water sources remains a primary concern for arid regions in both the developed and developing world. Climate change is causing fluctuations in the frequency and duration of precipitation, which can be seen as prolonged droughts in some arid areas. Droughts decrease the reliability of surface water supplies, which forces communities to find alternate primary water sources. In many cases, ground water can supplement the use of surface supplies during periods of drought, reducing the need for above-ground storage without sacrificing reliability objectives. Unfortunately, accessible ground waters are often brackish, requiring desalination prior to use, and underdeveloped infrastructure and inconsistent electrical grid access can create obstacles to groundwater desalination in developing regions. The objectives of the project are to: 1) mathematically simulate the operation of hollow fiber membrane distillation systems and 2) optimize system design for off-grid treatment of brackish water. It is anticipated that methods developed here can be used to supply potable water at many off-grid locations in semi-arid regions including parts of the Navajo Reservation.

This research is a collaborative project between Sandia and the University of Arizona. The algorithm research and computer code development, utilizing Sandia unique hardware, has broad applications and mission relevance to critical issues of energy security.



## Multiscale Multiphysics for Subsurface Science and Engineering of Shale

180869 | Year 2 of 3 | Principal Investigator: H. Yoon

### Project Purpose:

Nanoporous geomaterials such as shale and carbonate rocks are becoming an increasingly important rock type with emerging climate and energy security problems. However, there is no consensus as to fundamental mechanisms underlying observed rapid decline in gas production and the fate of fracking fluids in shale gas fields. Movement of CO<sub>2</sub> plumes in the subsurface through shale caprocks has not followed model prediction. Furthermore, nanoscale pore size, surface chemistry, and complex connectivity in shales result in unique flow properties in contrast to those in other rock types. Consequently, the response of anisotropic heterogeneous shale geomaterials to engineered 3D thermal, fluid flow, and stress perturbations are not currently quantifiable to a degree where prediction is viable.

In this project, we focus on multiscale analysis of nanoporous shale and carbonate rocks to gain a fundamental understanding of poromechanical and flow responses of low permeability rocks with broad compositional range and physical and chemical heterogeneity. Multiscale imaging techniques (dual focus ion beam-scanning electron microscopy (FIB-SEM) with 3D energy dispersive spectroscopy (EDS), x-ray micro-computed tomography, optical and laser confocal microscopy) are used to characterize pore structures and mineralogical distributions in nanoporous shale and carbonate rocks. These multiscale imaging results combined with neutron scattering analysis enable us to characterize hierarchical complexities in nanoporous geomaterials at an unprecedented scale and to account for the impact of chemical reaction on nanopore structures. Detailed pore-scale modeling of coupled micromechanics and fluid dynamics integrated with multiscale imaging and experimental testing will allow for direct correlation of upscaled flow and mechanical properties to upscaled chemical reactivity and poromechanical responses.

The result of these integrated approaches will be a science-based, rather than empirical, workflow for understanding and predicting fluid-rock interactions in nanoporous geomaterials that are crucial to emerging subsurface issues such as shale resources recovery, geological CO<sub>2</sub> storage, nuclear waste disposal, and induced seismicity.

## Nanocomposite Barrier Films for Enhanced Thin Film Photovoltaic Stability

180865 | Year 2 of 3 | Principal Investigator: E. D. Spoeke

### Project Purpose:

Long-term reliability, functional device lifetime, and consumer safety are central concerns for the cost-effective integration of photovoltaic (PV) systems in the rapidly evolving global stationary energy scheme. Failure or degradation of encapsulant coatings protecting sensitive PV materials and electronics from environmental moisture and oxygen is arguably the leading cause of PV degradation and failure. These failures affect reliable utility and introduce unacceptable maintenance and replacement costs. We will develop and evaluate a robust, low-cost, optically transparent, highly impermeable polymer-clay nanocomposite (PCN) thin film barrier/encapsulant technology. Currently, used glass barriers are expensive, heavy, and susceptible to cracking, while the current polymer encapsulants are temperature sensitive, subject to polymer degradation, and inadequate for long-term environmental (e.g., moisture) protection. Our alternative composite thin film barrier, comprising delaminated clay platelets, dispersed and oriented within a polyelectrolyte polymer matrix, is deposited using scalable layer-by-layer (LBL) processes. These composite thin films are transparent, flexible, conform to irregular shapes, and exhibit excellent oxygen/moisture exclusion. Moreover, known fire retardant properties of these oxygen barriers introduce unprecedented protection against fires caused by device arc-faults. By improving thin film PV stability and reliability, these nanocomposite encapsulants will impact national photovoltaic priorities while aligning closely with Sandia's ongoing focus on device reliability. Mating Sandia's strengths in materials development and PV reliability also promises expanded leadership opportunities within the renewable energy and more broadly in the photovoltaic community, while the barrier technology itself may impact additional national security mission space concerned with environmentally sensitive optics or electronics (e.g., satellites, nuclear weapons).

Novel PCN thin film PV encapsulants offer potentially high rewards, promising improvements in PV reliability, stability, and safety, all critical issues plaguing PV integration into the national electrical energy infrastructure. This project explores the feasibility of this approach, employing scientific study to inform system optimization and address risks associated with using these untested materials.



## Next Generation Global Atmosphere Model

173079 | Year 3 of 3 | Principal Investigator: W. Spatz

### Project Purpose:

To assess the national security implications of climate change, the US will need climate models that run efficiently on a multitude of emerging computing architectures and are capable of uncertainty quantification (UQ). No existing climate model possesses either of these capabilities, and modifying existing codes to attain them is daunting enough to warrant the development of new models that incorporate these capabilities from the start. A new global atmosphere model will be created that addresses these needs through calculated development of the existing Sandia software technologies Trilinos, Dakota, and Albany.

Emerging computing platforms are taking many different forms, and developing algorithms that exploit each form to maximum effect is a cutting-edge design goal called performance portability. Sandia has developed a strategy to achieve this goal, one supported by enabling code in the Trilinos suite of scientific software packages.

Uncertainty quantification is an emerging field of study within the computational sciences—closely related to optimization—and Sandia has developed the Dakota package to enable these capabilities. Dakota can treat existing science applications in two ways: as black boxes, or with more advanced algorithms that require embedded logic within the application.

Albany is an application development code base, built on top of Dakota and the many packages within Trilinos to provide rapid development of finite element scientific applications with access to cutting-edge computational capabilities. In this project, we used Albany to develop a state of the art global atmosphere model that is performance portable and can quantify uncertainty.

The results of this project will address regional refinement and UQ processes and tools in a new atmospheric dynamical core. We have demonstrated what is possible in a modern Earth system model, and provided the groundwork for using such a system model for enabling the mitigation of, or adaptation to, climate change impacts.

## Novel MEMS-Enabled Nanofracking of Subsurface Minerals

192762 | Year 1 of 3 | Principal Investigator: K. L. Jungjohann

### Project Purpose:

It has been estimated that by 2035, 45% of the US natural gas supply will come from shale gas, which is the second highest energy source in the US today. The process of harvesting natural gas from shale is accomplished by *fracking*, where high pressure water (with chemical additives) is used to open existing and create new fractures in the subsurface. Fracturing of rocks is predicted when stress conditions exceed critical values; however, local chemistry can dramatically lower the failure envelope for a variety of rock types (shale and limestone). This process is referred to as subcritical fracturing. While chemical effects have been documented, there is no mechanistic understanding of the exact chemical reactions at the fracture tip.

We hypothesize that subcritical fracture exerts first-order control on the permeability of shale during hydrofracking. Mesoscale characterization of the coupled chemomechanical processes at a fracture tip has not been achievable due to its atomic scale nature and environmental conditions (liquid under strain). To enable characterization, we will create a microelectromechanical system (MEMS) platform to recreate and control the environmental conditions, and integrate membrane windows for simultaneous atomic scale structural and chemical correlative imaging during fracturing within a transmission electron microscope (TEM). We have designed and initiated fabrication of a first-of-its-kind liquid-mechanical TEM MEMS device that will allow us to quantify the atomic scale structure at a fracture tip in shale minerals (mica, quartz, and calcite) during chemical attack.

In addition, we have developed ex situ liquid nanoindentation at Sandia to measure elastic modulus, hardness and indentation fracture, as well as stress/strain measurements of dry shale minerals using a TEM tension holder. These results will be coupled with surface charge measurements and dissolution rates of the minerals in a variety of chemistries (deionized water, fracking fluid, HCl [ranges of pH]) to provide a holistic understanding of the coupled chemomechanical control on shale fracture.





## Nuclear Power Plant Cyber Security Discrete Dynamic Event Tree Analysis

191054 | Year 1 of 2 | Principal Investigator: T. A. Wheeler

### Project Purpose:

Instrumentation and control of nuclear power is transforming from analog to modern digital assets. These control systems perform key safety and security functions. This transformation is occurring in new plant designs as well as in the existing fleet of plants as the operation of those plants is extended to 60 years. This transformation introduces new and unknown issues involving both digital asset induced safety issues and security issues.

Traditional nuclear power risk assessment tools and cybersecurity assessment methods have not been modified nor developed to focus on the unique nature of cyber failure modes and of cybersecurity threat vulnerabilities. This project is developing a dynamic cyber-risk informed tool to facilitate the analysis of cyber failure modes and the time sequencing of cyber faults, and to impose those cyber exploits and cyber faults onto a nuclear power plant accident sequence simulator code. The code will assess how cyber exploits and cyber faults could interact with a plant's digital instrumentation and control (DI&C) system and defeat or circumvent a plant's cyber security controls. This will be achieved by coupling existing Sandia nuclear accident dynamic simulator codes with a cyber emulotics code to demonstrate real-time simulation of cyber exploits and their impact on automatic DI&C responses.

Studying such potential time-sequenced cyber attacks and their risks (i.e., the associated impact and the associated degree of difficulty to achieve the attack vector) on accident management will provide a risk-informed basis for developing effective cyber security controls for nuclear power. Current approaches to cyber vulnerability have not adequately focused vulnerability and the efficacious identification of security controls for supervisory control and data acquisition (SCADA) DI&C systems. This project will bring Sandia's well established strengths in nuclear safety and cyber threats together to establish a unified cyber/nuclear hazard analysis modeling capability.

## Optimizing Microgrid Energy Delivery Under High Uncertainty

181202 | Year 2 of 3 | Principal Investigator: A. Ellis

### Project Purpose:

The power grid is evolving toward a more decentralized system. Distributed generation, storage, electric vehicles and load response (collectively distributed energy resources or DER) will increasingly be called upon to support grid reliability, as centralized generation does today. This project will explore the fundamental mathematical and engineering concepts required to establish a new "energy delivery" paradigm for the power grid. Under the "energy delivery" paradigm, bulk generation would deliver blocks of energy at negotiated prices. Consumers (residential, commercial, industrial, institutional), who ultimately control net power demand and DER, would assume responsibility for instantaneous power balancing. This model could potentially make the grid more sustainable, reliable, and efficient.

This is a difficult technical problem. It requires a substantial reformulation of the power system scheduling problem where security constrained unit commitment and optimal power flow are applied to optimally dispatch generation while maintaining adequate headroom for real-time control. Both Sandia and New Mexico State University (NMSU) are working on price-based schemes, for regulation and scheduling respectively. An investigation of the inherent uncertainty associated with load, generation, and the evolving grid including microgrids have been included in formulation, with encouraging results. NMSU has established a proof of concept for the deterministic and stochastic cases for small systems. The challenge is to demonstrate tractability at scale, including renewables or microgrid/smartgrid deployment with communications.

We plan to further demonstrate the energy delivery concept through a simulation in Matlab or Python, using realistic stochastic models for load, renewable energy generation, and market clearing price. Operations and maintenance, as well as reliability of generation assets, will be taken into account. We will also attempt to validate assumptions around load criticality. This project will develop a hardware implementation that showcases the energy delivery concept. The plan will consider the use of distributed resources currently in operation at Sandia's Distributed Energy Technologies Laboratory.



## Predictive Engineering Tools for Novel Fuels

173664 | Year 3 of 3 | Principal Investigator: M. P. Musculus

### Project Purpose:

This project investigates fundamental aspects of novel engine cycle performance, alternative fuel, and hydrogen combustion engineering through a partnership with the University of California Berkeley. The project aims to use the best combustion engineering tools available to explore methods for increasing efficiency and reducing the climate effects of energy utilization. For example, successful biofuel implementation may involve cooperative evolution of fuel discovery and engine innovation, which requires rapid but reliable means to assess the performance characteristics of novel fuels based simply on their molecular structure. This project will develop and expand predictive engineering models, employing artificial neural networks, and predictive data analysis tools to infer quantitative structure-performance relationships. These relationships will serve as a first sorting tool for more detailed and fundamental structure activity investigations.

Other investigations will focus on novel ways of efficiently utilizing noncarbon energy carriers such as hydrogen, thereby developing new engine cycles that will dramatically improve efficiency. For example, using a noble gas as the working fluid in a closed-loop internal combustion engine cycle could potentially offer substantial improvements in efficiency, but substantial modeling of modifications to the engine cycle is required, as well as development of test engines. The Berkeley group will model and develop these tools in collaboration with Sandia scientists.

## The Effect of Proppant Placement on Closure of Fractured Shale Gas Wells

173076 | Year 3 of 3 | Principal Investigator: M. D. Ingraham

### Project Purpose:

Production declines in hydraulically fractured shale gas wells are higher than conventional wisdom predicts and resulting long term gas yields are low. A science-based approach to understanding proppant flow and proppant-formation interaction could yield new technologies that extend well life while better protecting the environment. Well restimulation (e.g., pumping acids to dissolve clogging debris or refracturing the formation) can help with this problem, but is costly and involves additional water use and is environmentally detrimental. The declining cost of oil has resulted in a drop in the number of new wells being drilled. This increases the need for better extraction from both existing and new wells, as it is more difficult to drill a financially viable well. However, for the security of the US energy economy, it is critical that all energy resources are exploited to their fullest. A better solution would involve improvements to the original hydraulic fracturing and proppant injection process.

Laboratory-scale fracturing experiments were coupled with proppant flow modeling utilizing multiphase flow models to determine the effect of proppant placement on the ability to keep formation permeability high. The mechanical tests and resulting CT scans of samples were used to inform model development and parameterization. Models were then run to determine optimum proppant densities within a fracture in terms of both stability of the proppant pack and permeability of the fracture.

There is little published work on this type of work because much of the results from industry are considered trade secrets. The published work is on simplistic models and tests performed between flat plates, without natural variation or under unrealistic stresses. This work utilizes actual fracture geometries, developed from CT scans, and tests performed under representative stress states.



## The Role of Real-Time Decision Making in Grid Resilience

173078 | Year 3 of 3 | Principal Investigator: L. Burnham

### Project Purpose:

The transformation of the distribution grid from a centralized to decentralized architecture, with bidirectional power and data flows, is made possible by a surge in network intelligence and grid automation. While this transformation is largely beneficial, moving the nation closer to the concept of a self-healing grid, the interface and codependencies between grid operator and automation are not well understood, nor are the benefits and risks of automation, particularly during high-stress outage events. Quantifying and understanding the latter is an important facet of grid resilience that needs to be fully investigated.

The project aims to identify and mitigate the vulnerabilities posed by automation for a grid that will remain a human-in-the-loop critical infrastructure for the foreseeable future. To that end, we intend to identify the causal relationships between operator performance and automated technologies and to measure human performance as a function of automation.

Our multifaceted, multidisciplinary approach, which has experimental research at its core, is pioneering for the domain. Our short-term goal is to bring national attention to what we believe is a largely unrecognized but critical facet of grid resilience; our ultimate goals are to leverage our experimental methodology and analytical framework to build an extensible platform for more deeply investigating the human dimension of grid reliability and resilience.

## Understanding Photo-induced Oxidation Mechanisms of Volatile Organic Compounds

176312 | Year 3 of 3 | Principal Investigator: D. L. Osborn

### Project Purpose:

Understanding of the oxidation mechanisms of volatile organic compounds (VOCs) in the troposphere is crucial to human health. Atmospheric modeling relies on well-known oxidation mechanisms to interpret the changing global environment and assess the health risks associated with climate change. Oxidation of VOCs leads to the formation of photochemical smog, yet insufficient data exists on the initial oxidation steps that occur in polluted and pristine environments, especially at temperatures relevant to the atmosphere. We recently developed a low-temperature flow reactor that is used in conjunction with the Multiplexed Photoionization Mass Spectrometer to directly probe chemical reactions as they occur at atmospherically relevant temperatures. In addition, we have measured the absolute photoionization cross sections of four molecules key to both atmospheric and combustion chemistry: water, hydrogen peroxide, formaldehyde, and hydroxide. These cross sections will be used in further DOE funded studies. The larger temperature range now available will be directly applicable to tropospheric chemistry, and provide a more rigorous test of radical-radical associations important in combustion chemistry.

The Criegee Intermediate (CI) forms during hydrocarbon oxidation in the atmosphere; until recently, its reactivity with other atmospheric species was largely unknown. The reaction of CI with ozone has been theorized to be fast; however, the rate has not been measured experimentally due to the complex nature of this chemical system. Using the Sandia Broadband Cavity Enhanced Absorption Spectrometer, we are directly measuring the CI + ozone reaction rate. Preliminary results suggest that this reaction is indeed fast.

This project investigates fundamental chemistry relevant to atmospheric sciences through a partnership with the California Institute of Technology. This research seeks to quantitatively measure oxidation reaction rates at relevant temperatures. If successful, this innovation would place models of smog formation on a more sound scientific footing and increase fidelity of model predictions. The key impact of the project will be in developing better predictive models of combustion and atmospheric chemistry, both DOE mission goals.



## Validating Hydrogen Concentration Fields at Crack Tips

186839 | Year 2 of 3 | Principal Investigator: J. A. Ronevich

### Project Purpose:

Gaps remain in fundamental mechanistic understanding and modeling of hydrogen embrittlement, presenting an opportunity to fill these gaps through application of advanced analytical techniques. Despite notable progress in developing predictive models (e.g., recognizing that robust models must couple the crack-tip fields with a material damage criterion), uncertainty remains in quantifying the stress fields surrounding a crack tip. This uncertainty, in turn, affects the predicted hydrogen concentrations ahead of crack tips, since these concentrations are dependent on the magnitude of hydrostatic stresses. To date, hydrogen concentration predictions have not been validated through experimental measurements. The goal of this project is to measure hydrogen concentration fields at crack tips to validate the magnitude of the hydrogen field, and concurrently infer the form of the stress field. Advanced predictive models for hydrogen-assisted cracking currently rely on adjustable parameters to correct for uncertainty in the crack tip stress field and its associated hydrogen concentration field. Our approach is to introduce hydrogen into statically loaded specimens through gaseous and electrochemical charging. Several highly sensitive analytical techniques—[nuclear reaction analysis (NRA) and kelvin probe force microscopy (KPFM)]—will be employed in parallel to measure hydrogen concentrations ahead of crack tips with submicron level resolution. Quantifying hydrogen concentrations with high resolution near crack tips will improve our understanding of hydrogen embrittlement mechanisms and inform predictive models, thereby reducing design margins for structural components.

The project focuses on fundamental science directed at measuring hydrogen concentration fields at crack tips with high fidelity for the first time. Quantifying the magnitude of the hydrogen concentration field and concurrently inferring the form of the stress field will inform and enhance the development of predictive hydrogen-assisted cracking models applied to materials and components in energy technologies.

## Waste Water for Power Generation via Energy Efficient Selective Silica Separations

191018 | Year 1 of 2 | Principal Investigator: T. M. Nenoff

### Project Purpose:

Thermoelectric power generation is the largest user of freshwater in the US, at *~500 billion gallons/day, which is almost half of all water withdrawn daily*. Replacement of that freshwater with purified oilfield produced waters, municipal or agricultural wastewaters, and subsurface brines is possible only if dissolved silica and calcite are prevented from forming mineral scales during the power generation process. Existing anti-scalant technology can already prevent calcite buildup. However, there is no low energy method for preventing silica scaling, thereby limiting the amount of impaired water recycling that can be achieved. Dissolved silica is ubiquitous in impaired waters, resistant to existing anti-scalants, and difficult to remove from power plant feedwaters. This project is focused on developing silica getter materials that will be tested at the field and pilot scale.

Our project is both an innovative approach for developing high silica capacity and selectivity solid sorbent materials, and is cutting edge for collaboratively: 1) developing novel materials and their processes for silica removal, with the use of 2) technoeconomic modeling and analysis to aid in real-world implementation. We will build upon our unique experiences in low energy desalination and silica removal screening tests to ensure success.

This project addresses an industry-wide research problem. Existing dissolved silica removal methods are ineffective, energy intensive, negatively impact the environmental, and generate high volume sludges/brines. Developing new separations media that remove dissolved silica directly lowers the energy penalty of water treatment, is applicable to large volume produced waters, and allows substitution of impaired waters into many energy production scenarios worldwide.



## Water Treatment System for Resilient Energy Production

191051 | Year 1 of 3 | Principal Investigator: L. Biedermann

### Project Purpose:

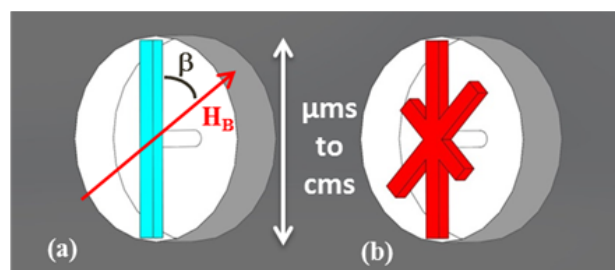
Low-energy, high-flux desalination membranes would be an enabling technology both for energy generation (increase power plants' resiliency by increasing the cycles of water recirculation in cooling towers) and for energy production (treating produced water from hydraulic fracturing for productive reuse). Revolutionary water treatment systems for energy production would operate at energy intensities  $<2 \text{ kWh/m}^3$  and have high chemical tolerance. An ideal desalination membrane provides desalination via ion exclusion, drives low-energy permeation, resists organic contaminants, and tolerates chlorine (biofouling mitigation).

Our graphene oxide (GO)/polymer membranes comprise three key layers: 1) the laminar GO provides ion rejection via the thin-slit permeation pathways, 2) the covalent linker molecules ensures membrane integrity, and 3) the porous polymer support provides mechanical durability and allows for scale-up to larger membrane sizes. The project will address two science questions that drive GO/polymer membrane development: "What materials ensure robust, scalable membranes?" and "What mechanism drives low-energy permeation?"

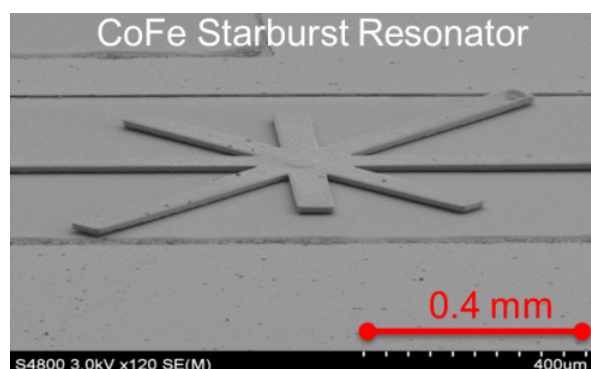




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**a) Single frequency resonator**  
**b) Multi-Frequency resonator (3)**



## International, Homeland, and Nuclear Security

A vital US national security concern is that various adversaries who want to acquire power, support, and legitimacy are attracted to weapons based on nuclear, radiological, chemical, biological, cyber and explosives threats, or some combination of these threats. As the threat becomes more sophisticated and creative, we must identify effective solutions that mitigate current and future risks. The International, Homeland, and Nuclear Security IA invests in research that enables creative solutions in international and domestic risk reduction against these threats. Note that the this IA was re-named Global Security beginning in FY2017.

*The image above shows a conceptual rendering of a single-frequency/multi-frequency magnetic smart resonator next to a real microfabricated version. This is a first-of-its-kind electroformed magnetoelastic resonator structure. Development of these types of "smart structures" is critical for both treaty verification and safeguards to establish and track the identity of accountable items. (Project 180893, Magnetic Smart Tags (MaST) for Arms Control and Treaty Verification)*

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## A Complex Systems Approach to More Resilient Multi-Layered Security Systems

173114 | Year 3 of 3 | Principal Investigator: N. J. Brown

### Project Purpose:

In July 2012, protestors cut through security fences and reached the exterior of the Highly Enriched Uranium Materials Facility at the Y-12 National Security Complex. This was believed to be a highly reliable, layered security system. The configuration of layered security measures is at the center of efforts to protect a range of systems from high-value facilities to large-scale infrastructures.

Historically, analyses of security systems have been performed using directed graph and path analysis tools like Adversary Sequence Diagrams (ASD). However, there are many dimensions in the design space of a security system, including selection of technologies, alternative locations/configurations, different threats, and competing cost limitations. The dimensionality of this problem makes it effectively impossible to evaluate all permutations of potential system architectures using traditional methods. The experience of the individuals configuring the system drives the careful examination of a small subset of architectures.

The key goal of this project is the creation of a consistent, robust mathematical framework using complex systems analysis algorithms and techniques to better understand the emergent behavior, vulnerabilities, and resiliency of layered security systems subject to budget constraints and competing security priorities. Because there are several dimensions to security system performance and a range of attacks that might occur, the framework must be multi-objective for a performance frontier to be estimated. Since security measures can fail for a range of reasons, this research will also explicitly include resiliency as a dimension of system performance.

To extend beyond traditional methods, innovative modeling of multi-layered security systems requires a complex system approach which integrates multiple dynamic and stochastic algorithms, including an optimization model for automatically generating security architectures. This project develops a rigorous computational framework, flexible enough to apply to a range of layered security system design instances, including complex system behaviors like emergence and resiliency.

## Advanced Imaging Algorithms for Radiation Imaging Systems

173669 | Year 3 of 3 | Principal Investigator: P. Marleau

### Project Purpose:

Radiation imaging devices are important to the nuclear security and safeguards communities due to their ability to detect and localize radioactive sources. Because of their low natural background, difficulty to shield, and unique association with special nuclear material (SNM), fast neutron imaging provides a promising means for the detection of SNM. To make these systems useful for end-user applications, robust reconstruction and analysis algorithms must be developed that provide detailed information on the location, energy spectrum, and intervening material. To date, deconvolution, match filtering, and maximum-likelihood expectation-maximum (MLEM) have been demonstrated. However, the information provided is limited to an approximate location of the source.

The intent of this work was to develop the algorithms that will bring the analysis from qualitative images to quantitative attributes of objects containing SNM. The first step to achieving this was to develop an in-depth understanding of the intrinsic errors associated with the deconvolution and MLEM algorithms. Toward that end, significant effort went into developing bootstrap methods for estimating statistical uncertainties and experimentally validating them.

These methods were exercised on University of Michigan's Dual Particle Imager (DPI) to demonstrate that simultaneous reconstruction of fast neutron and gamma-ray images and spectra can be made quantitative. The results were then used to evaluate potential sources of systematic uncertainty. As a final proof of concept, we analyzed data taken from a very complex environment. The DPI was able to successfully locate and identify a SNM sample in a field of view (FOV) that also contained other shielded and unshielded radioactive sources. The non-SNM sources were also correctly located and identified.



## Applying Biological Immune-System Concepts to Improve Electronic Biosurveillance System Performance

191183 | Year 1 of 3 | Principal Investigator: P. D. Finley

### Project Purpose:

This project will improve the ability of electronic biosurveillance (EBSV) systems to rapidly identify bioattacks and emerging disease outbreaks. Today, operational EBSV systems rely on traditional statistical methods or keyword searches to detect patterns in data that indicate the presence of bioterrorism agents or emerging pathogens. These detection methods struggle to cope with baseline data that are noisy and vary through time. We propose to address these limitations by developing a data-fusion architecture that classifies anomalies by combining patterns from multiple observed data streams.

The proposed data fusion will use artificial immune systems (AIS) algorithms to classify patterns of responses of online anomaly detectors as they monitor multiple syndromic data feeds. We will test its effectiveness on: 1) a simulated anthrax attack in the San Francisco Bay Area—to test against a nonstationary baseline and 2) the 2009 swine flu outbreak—to test against a novel pathogen. The system will be validated rigorously to determine its potential for improving the performance of operational EBSV systems, thus improving the Nation's capacity to detect and respond to potential biosecurity events. Both the algorithmic and architectural strategies proposed to address these challenges represent significant departures from current practice.

This research takes a radical approach to addressing longstanding challenges to EBSV system effectiveness. Previously, neither AIS methods nor ensemble classification have been applied to specific limitations of production EBSV systems. This composite architecture promises to excel at handling this nonstationary online learning problem.

## Arming and Firing System Charge State Determination using Unintended Radiated Electromagnetic Emissions (URE)

191150 | Year 1 of 3 | Principal Investigator: J. T. Williams

### Project Purpose:

The purpose is a fundamental investigation into electromagnetic unintended radiated emission (URE) and propagation mechanisms from capacitive discharge firing systems to inform the future development of a broadband radio frequency (RF) diagnostic tool to *remotely* identify the instantaneous charging state of a firing system. Primary emphasis will be placed on entirely *passive* collection approaches. Secondary to this effort is a fundamental investigation into the application of *active* RF interrogation techniques with special emphasis on identification of peripheral components commonly found in relevant arming and firing systems.

The feasibility of exploiting passive URE to detect the high voltage charging circuitry of capacitive discharge firing systems has been demonstrated empirically. However, there is an inadequate and incomplete understanding of the fundamental radiation sources and emission mechanisms that may be available for exploitation. As a result, existing approaches have limited sensitivity, stand-off, interference immunity, selectivity (high false alarm rate), and require more exquisite operator expertise than is likely necessary. We propose to develop a more fundamental understanding and new robust detection and classification techniques of a variety of potentially exploitable URE sources and emission mechanisms.

An element of the proposed effort is to investigate the feasibility of remotely detecting low-level “partial discharge” phenomenon known to be present inside of charged high voltage capacitor dielectrics. While very high risk, it is conceivable that this approach could be used to enable the remote detection of a charged high voltage capacitor in complete isolation from any associated high voltage charging circuitry—a task currently considered impossible.

Previous related efforts have focused on developing tools to detect a limited subset of potentially exploitable phenomena. A comprehensive investigation of URE sources and radiation mechanisms is required to establish fundamental understanding to exploit these signatures. This fundamental research and development effort is not yet mature enough for NNSA or DoD investment.





## Automated Discovery in Emulytics

180889 | Year 2 of 2 | Principal Investigator: D. J. Fritz

### Project Purpose:

Our nation's critical infrastructures depend on distributed information systems, which must be resilient against malicious attempts to disrupt their operation. Security mechanisms must be deployed and continuously assessed in order to prevent adversaries from disrupting critical infrastructure. These information systems employ a broad range of technologies including fixed Ethernet, point-to-point wireless, and cellular communications. Additionally, these systems employ enterprise architectures, cloud-based data centers, and emergency response wireless architectures. With the extensive reliance of critical infrastructure on secure information systems, techniques and mechanisms to assess security must be created.

Efforts to extend state-of-the-art security modeling via emulation capability are hindered by our current ability to model meaningful emulations of real-world networks. To date, emulation research has focused on the means and mechanisms of emulation with little emphasis on fidelity or representative behavior of experiments. We propose to create a method to conduct information system discovery and develop tools to enable the creation of high-fidelity emulation models that can be used to enable assessment of our infrastructure information system security posture and potential system impacts that could result from cyber threats. In addition, this work will help gauge the fidelity of the constructed emulation model, which is critical in providing confidence in research questions answered on this platform. Providing confidence and fidelity in emulation experiments is fundamental to addressing current and future US cybersecurity missions. This research will impact the landscape of research in large scale emulation, and enable addressing critical research areas that can only be answered using a high fidelity emulation platform.

## Automated Generation of Tailored Malware Execution Environments

191162 | Year 1 of 2 | Principal Investigator: C. Shannon

### Project Purpose:

Cyber defenders often employ automated dynamic analysis to uncover malicious functionality in an unknown executable. However, in many cases, malware will only reveal its true functionality when executed in its target environment. For example, Stuxnet only compromised machines before June 24, 2012. As a result of environment specific triggers, defenders must invest significant time to manually identify the required environment and malicious functionalities.

We propose a novel system to quickly and automatically discover the target environment for a given executable based on virtual machine introspection (VMI). Specifically, our approach will be two-fold: 1) develop a novel, covert technique for tracing Windows processes at the application programming interface (API) call level based on VMI and 2) integrate these results with a contextual understanding of Windows to dynamically generate virtual machines tailored for a specific sample of malware.

If successful, this project will create a new class of dynamic analysis systems to uncover previously unseen behavior in malware found across the US government. Cyber defenders will benefit from a system that automatically provides a detailed execution trace and the execution environment that elicited the executable's malicious behavior. In addition, this system would create virtual machines containing malware "primed" for execution that would greatly enhance Emulytics™ experiments.

Existing research focuses on techniques that are either too fine-grained (central processing unit instruction traces) or too coarse-grained (system call traces) to fully infer the malware's target environment. By transparently monitoring at the Windows application program interface (API) level, we can better understand malware intent and provide more meaningful information to the analyst.



## Biosecurity through Public Health System Design

198564 | Year 1 of 1 | Principal Investigator: W. E. Beyeler

### Project Purpose:

Effective response to bioweapon attack and emerging pathogens will rely upon a resilient public health infrastructure. Robust health systems serve to contain biological events, effectively reducing the likelihood of spread. Current efforts to strengthen health systems are often disorganized and inefficient, creating underutilized capacity with dual use potential. This project will apply sophisticated modeling and analysis methods to improve surveillance, and consolidate and reduce dual use technologies and materials.

Outbreaks of serious communicable diseases are becoming more common as the global population continues to grow and become more mobile. In addition to tragic consequences for the affected regions, disease outbreaks can result in global spread, and challenging global health security. Currently, public health networks in many countries do not function properly. Facilities for monitoring, laboratory testing, and treatment are usually designed and managed by disparate external organizations with narrow focuses and short attention spans. Often, countries are left with a hodgepodge of equipment and expertise that is poorly matched to the needs of the local population. Besides producing inadequate health benefits for the amount of money spent, this process can result in the proliferation of dual use capabilities, facilities, and equipment that present significant security risks. Systematically strengthening public health systems would benefit national security by strategically allocating resources and designing sustainable public health networks capable of responding to global disease threats.

Systematic optimization of public health resources is an innovative approach to improving biosecurity. New models predicting medical service demand given disease characteristics and resource distribution are needed. Stochasticity and extreme uncertainty call for novel quantification techniques that will be developed in this project.

## Building the Scientific Basis for Cyber Resilience of Critical Infrastructure

179224 | Year 3 of 3 | Principal Investigator: M. J. Hutchins

### Project Purpose:

The goal of this work was to develop a framework for understanding resilience metrics to serve the purpose of improving cyber resilience in critical infrastructure (e.g., energy systems). Through this research, we developed new mathematically rigorous algorithms and models for quantifying, measuring, and increasing the cyber resilience of critical infrastructure. Vulnerabilities in the existing global digital information and communications infrastructure (i.e., "cyberspace") may be exploited by an adversary, which places critical US systems at risk (e.g., financial, energy, transportation, and security). The number of vulnerabilities is large and increasing in number, the attack surface is changing over time, and the problem includes technical and nontechnical factors. Given this complex and dynamic landscape, mitigating risk is an important strategy. It is necessary to ensure that critical infrastructure is resilient, that is, able to efficiently reduce both the magnitude and duration of the deviation for targeted system performance levels.

Scientifically rigorous approaches to addressing cyber resilience are in the nascent stages; further research is required to develop the algorithms that accurately represent the full complexity of real world systems and threats. This effort focused on researching and developing models to facilitate the design of resilience enhancing countermeasures for specific critical infrastructure (CI) (e.g., energy delivery systems). We identified operational and design factors that affect cyber resilience of CI, and created systems models that represent dynamic interplay between these factors and the cyber threats that CI faces.



## Compressive Optical Physical Unclonable Function for Secure Communication

191185 | Year 1 of 2 | Principal Investigator: G. C. Birch

### Project Purpose:

Physical unclonable functions (PUFs) are tools used in cryptography to create easily observed, but difficult to predict, outputs tied to the physical properties inherently unique to a particular device. Most PUF technology has focused on electrical systems, but these require the presence of embedded electronics. Alternative PUFs that rely on macroscale interactions from optical effects, making them simpler to measure, have been explored. However, these optical PUFs are expensive and bulky, and have traditionally required coherent illumination (i.e., lasers). A PUF is needed that can be utilized where electronic PUFs cannot, or in applications where custom embedded electronics are not available, all while using cost-effective components.

We investigated a prototype device that utilizes an optical system to create a small, inexpensive, and easily manufactured compressive optical PUF (COPUF). This device utilizes the principles of computational imaging to miniaturize and simplify the optical PUF design and to increase robustness to outside environmental changes.

To develop this system, software and hardware elements are being explored. Ray trace software has been developed that allows for physically accurate simulation, design, and optimization of computational and compressive imagers like the COPUF. Closed-loop, full system simulations were developed that show the feasibility of the COPUF calibration and operational methods. Hardware prototypes were created that utilize 3D printed, transparent random scattering elements. COPUF prototypes capable of reconstructing scattered output data back into input messages were demonstrated with low bit error.

Realization of this project has numerous potential national security applications, including use in drone systems to both send and receive secure information, sending high consequence commands securely, and integration into trusted systems. Utilization of the computational and compressive image simulation capabilities developed in this project could lead to the development of novel imagers and other remote sensing devices.

## Decontamination of Radiological Contaminated Materials using Magnetotactic Bacteria

173106 | Year 3 of 3 | Principal Investigator: M. D. Tucker

### Project Purpose:

Decontamination of radiologically contaminated materials is a difficult task. Unlike toxic chemicals or biological organisms, which can be neutralized or killed, radiological contaminants must be physically extracted from a material. The objective of this project is to develop a novel approach using magnetotactic bacteria (MTBs)—bacteria that contain small magnetic structures—to decontaminate materials that have been contaminated with radionuclides such as cesium. MTBs have the capability to bind to and/or adsorb radionuclides. After deployment of MTBs onto a material, the bound radionuclide can then be extracted from contaminated materials using separation techniques that utilize the magnetic properties of the bacteria. In order to develop a system for radionuclide decontamination utilizing MTBs, four objectives must be demonstrated including: 1) identify, select, and culture an MTB strain with magnetic properties, 2) demonstrate that the selected MTB strain is radiation tolerant, 3) demonstrate that the magnetic properties are maintained in the selected MTB strain and can be used to extract the bacteria from a material, and 4) demonstrate that the selected MTB strain will uptake and/or sorb radionuclide contaminants. We have successfully achieved the first three objectives and significantly improved culturing methods for MTBs. In addition, we also successfully demonstrated genetic modification of MTBs. Efforts toward demonstrating uptake/sorption of a radionuclide (i.e., the fourth objective above) were partially successful—the MTBs only sorbed cesium at low levels, although significant uptake and sorption of other contaminants has been demonstrated by other researchers. Further development of this concept to achieve higher sorption of cesium and other radionuclides has the potential to reduce the need for removal and disposal of contaminated material surfaces and to increase resilience to disruptive radiological contamination events.



## Development of a Novel Nanoparticle Delivery Vehicle for Pre-Treatment with Nerve Agent Countermeasures

173110 | Year 3 of 3 | Principal Investigator: C. E. Ashley

### Project Purpose:

Nanotechnology promises to revolutionize prevention/treatment of organophosphorus (OP) nerve agent poisoning through encapsulation of nerve agent countermeasures in nanoparticles that improve their in vivo effectiveness. Two primary classes of nerve agent countermeasures are OP scavengers—proteins that directly bind or hydrolyze nerve agents—and acetylcholinesterase (AChE) reactivates—small molecule drugs that reverse the effects of nerve agent poisoning in the central nervous system (CNS). Chemical strategies for enhancing the efficacy of these countermeasures in rodent models have thus far failed, leading researchers to investigate nanoparticles that improve the circulation times of OP scavengers and deliver AChE reactivators across the blood-brain barrier. However, many existing nanoparticle delivery vehicles, including liposomes and polymerosomes, suffer from limited capacities, uncontrollable release profiles, and complex, specialized synthesis procedures that must be readapted for each new cargo molecule, leading to drug- and disease-specific ‘one-off’ approaches. To address these limitations, we propose to develop mesoporous silica nanoparticle-supported lipid bilayers (‘protocells’) for encapsulation and controllable delivery of OP scavengers and AChE reactivators. Protocells are potentially a ‘game-changing’ technology because their porous silica core and lipid shell can be modulated independently, which allows us to solve limitations of other nanoparticle delivery vehicles. We will demonstrate that protocells can be loaded with high concentrations of OP scavengers and AChE reactivators, administered to rodents via Sandia-developed polymer microneedles, and achieve either broad, systemic distribution or targeted accumulation within the CNS in order to prevent or reverse effects of poisoning by G-series and V-series nerve agents. Further, we will demonstrate that protocells protect rodents from lethal challenge with G-series and V-series agents when administered prophylactically (i.e., in advance of nerve agent exposure).

## Distributed Session Types for Trusted Systems and Communications

180921 | Year 2 of 2 | Principal Investigator: G. C. Hulette

### Project Purpose:

Distributed systems connecting groups of servers and weakly trusted clients while intermixing varying information sensitivities are becoming increasingly important. These systems provide a good opportunity for engineering-out of dangerous behavior, the design-in of levels of assurance, and dynamically detecting malicious changes. As an example, consider a set of servers with different chunks of sensitive data orchestrating provision of a service through the internet to multiple clients that may be untrusted or may be trusted via a trusted computing platform. Each server contains pieces of data that have different protection needs and a collection of mobile clients that may be untrusted or trusted. We proposed addressing three problems: 1) services provided by servers may be used by clients without correct permissions, 2) malicious clients may not be detected, and 3) statically allocated authorization may encourage either underpermissioning or overpermissioning.

In collaboration with the University of Illinois at Urbana-Champaign, this project investigated the use of session types as an extension to a functional programming language to make the language safer for concurrent programs. The results show how session types might be used in practice by realizing them in a language called SILL, and demonstrated several example programs in SILL where key concurrency properties (no deadlocks, etc.) are statically verified by the compiler. The work shows how to implement SILL in a variety of different language paradigms, including both a “standard” functional language (OCaml) and one equipped with dependent types (Idris).

The results demonstrate, in principle, how new programming languages could be created in which concurrent runtime errors such as deadlock would be statically eliminated. Concurrent programming is important to many areas of interest, including high performance computing and simulation. Verified safety of such programs would provide a useful baseline for higher level verification.



## Dual-Particle Imaging System with Neutron Spectroscopy for Safeguard Applications

180897 | Year 2 of 3 | Principal Investigator: T. M. Weber

### Project Purpose:

International safeguard efforts are key to ensuring a world that is not threatened by nuclear weapons. Since using nuclear technology for peaceful purposes is a right of every nation, monitoring nuclear facilities such as enrichment and reprocessing plants with material accountancy is critical to ensure that nuclear material is not diverted. Noninvasive techniques such as radiation detection are preferred to allow for inspections that do not interfere with facility operations. However, such nondestructive assay techniques must provide robust conclusions or they are of limited use. In collaboration with the University of Michigan, this project is investigating a spectroscopic radiation imaging system that is sensitive to both neutrons and gamma rays for safeguard applications such as design information verification and enrichment verification. Such a system will enable more accurate and robust verification of declared materials and activities.

## Electromagnetic (Optical/RF) Signatures Associated with Atmospheric Discharges and Plasma Generation in Explosive Events

195868 | Year 1 of 3 | Principal Investigator: R. Tang

### Project Purpose:

The detection and identification of explosive events is critical to meeting Sandia's future weapon and nonproliferation mission needs. The objective of this project is to increase the understanding of potentially unique characteristic electromagnetic phenomena associated with plasma generation and/or pre-plasma generation events. Leveraging existing plasma capabilities, this project seeks to develop experimental plasma generation and diagnostic methods to increase our understanding of both the unique signatures associated with explosive and nonproliferation processes and the potential ability to detect explosive events remotely using plasma related signatures. In addition, this work aims to increase the likelihood of event identification, and to probe the physics mechanisms underlying electromagnetic signals generation that can be tied to specific plasma/discharge processes. The primary goals of the proposed work are to study signatures from various chemical plasmas using different generation methods such as laser ablation and arc generation. In addition to explosive diagnostics, insights gained and techniques developed can likely be applied to areas of research related to component breakdown that could further lead to future diagnostics to predict device failures.

The work proposed is the first known dedicated effort to characterize optical/radio frequency signatures associated with both discharges and plasma generation from an explosive event. This work will: 1) advance our understanding of bulk explosive characteristics, 2) mature modeling capabilities through investigation of underlying physics mechanisms, and 3) potentially lead to a new detection paradigm.





## Enabling Explosives and Contraband Detection with Neutron Resonant Attenuation

186363 | Year 2 of 3 | Principal Investigator: M. Sweany

### Project Purpose:

Material Identification by resonant attenuation is a technique that measures the energy-dependent attenuation of 1-10 MeV neutrons as they pass through a sample. Elemental information is determined from the neutron absorption resonances unique to each element. With sufficient energy resolution, these resonances can be used to categorize a wide range of materials, serving as a powerful discrimination technique between explosives, contraband, and other materials. Our system is unique in that it simultaneously down-scatters and time tags neutrons in scintillator detectors oriented between a deuterium-tritium (DT) generator and sample. This allows not only for energy measurements without pulsed neutron beams, but for sample interrogation over a large range of relevant energies, vastly improving scan times. This system offers the potential to provide a breakthrough ability to provide detection discrimination of threat materials by their elemental composition (e.g., water vs. hydrogen peroxide) without opening the container. However, the technical and computational challenges associated with this technique have yet to lead to a fieldable technology. There are several open questions: what is the sensitivity to different materials, what scan times are necessary, what are the sources of background, how do each of these scale as the detector system is made larger, and how can the system be integrated into existing scanning technology to close current detection gaps? In order to prove the applicability of this technology, we will develop a validated model to optimize the design and characterize the uncertainties in the measurement, and then test the system in a real-world scenario.

This project seeks to advance the technical readiness level of this technology from laboratory tests that demonstrate proof of concept (TRL 3) to establishing an integrated system and evaluating its performance (TRL 4) through both laboratory tests and a validated detector model. The validated model will allow us to explore our technology's benefits to explosive detection for national security applications.

## Exploring Growth Conditions to Identify, Quantify, and Reduce the Risk of False Negatives

188289 | Year 2 of 2 | Principal Investigator: M. Finley

### Project Purpose:

The purpose of this project is to evaluate the BaDx (*Bacillus anthracis* diagnostic) device for potential false negative results. False negatives are extremely detrimental to the functionality of the assay, and can trigger accidental exposures, and possibly result in human deaths. Characterization and reduction of false negatives requires analysis of bacterial contaminants from clinical samples that grow in the device's microculture chamber that is designed to select for *B. anthracis*. Further, studies must be completed to quantify and characterize the growth of *B. anthracis* in selective growth medium within the BaDx culture chamber vs. standard culture conditions. The described microculture chamber is fundamental to the success of the device, and is the first of its kind. Understanding these growth conditions and factors that affect it will eliminate nearly all false negatives.

Solutions and corrective actions will be identified and implemented to significantly reduce (or eliminate) false negatives. Specifically, improving conditions for *B. anthracis* growth and production of target antigen within the BaDx culture chamber will be explored. This includes addition of rapid germination chemistry to the selective growth medium to facilitate rapid growth, as well as addition of other media constituents to improve growth while restricting growth of other potential bacterial contaminants. Additionally, the impact of the microculture chamber materials (plastics, adhesives, neodymium magnets) on *B. anthracis* growth, production of the target protein analyte, and interactions of the materials with the target protein will all be quantified. If successful, the BaDx device will be ready to send to the US Center for Disease Control for evaluation.



## Eyes on the Ground: Visual Verification for On-Site Inspection

191161 | Year 1 of 3 | Principal Investigator: M. McDaniel

### Project Purpose:

On-site inspection of nuclear facilities is arguably the most important tool for early detection of proliferation activities. However, inspectors are ill-equipped to detect a large portion of proliferation indicators. Many nuclear fuel cycle indicators are detectable by exclusively observational means; no radiological or chemical means exist for detecting some indicators. However, there exists no currently available technology to assist the inspector in detecting these observable indicators. Such technology would greatly improve the inspector's ability to detect proliferation activities in the field. Advances in imagery analysis, computer vision, and semantic data analysis have the potential to ease the inspector's cognitive burden by extracting actionable information from imagery and other sensor data. Observational inspection activities, such as counting  $UF_6$  cylinders in enrichment plant storage, determining precise dimensions of large equipment, or identifying uncommon equipment, is often difficult and time consuming.

This work is developing technology to automate and/or assist repetitive, and time-consuming observational inspection tasks by drawing upon commercially available sensing platforms, custom analysis software, and leveraging existing Sandia capability in semantic graph-based image analysis. The resulting advances will prove useful in other important nonproliferation and commercial domains.

We hypothesize that, with appropriate data, semantic graph-based object detection analysis can provide additional capabilities to on-site inspectors to improve their ability to detect visual and observational phenomena during inspections.

## Geospatial Nonproliferation Signature Modeling

198372 | Year 1 of 1 | Principal Investigator: M. D. Clemenson

### Project Purpose:

This project was meant to improve flow transport models and optical simulations of dispersed plume phenomenology. Geometries of facilities with plume emission were created in 3D to be used for modeling in the Sandia-developed SIERRA/Fuego reacting flow simulation code. Laboratory experiments using thermogravimetric analysis and gases of interest were performed to improve the fidelity of simulating interactions between the plume gas and nearby structure surface materials. A variety of surface materials were tested throughout the laboratory experiments in order to inform the Fuego code. Many of these surface material interactions have previously not been modeled in Fuego to our knowledge.

The optical simulations were performed in the Digital Imaging and Remote Sensing Image Generation (DIRSIG) software. A more advanced plume model was developed in DIRSIG by implementing specific gas spectral information that was not previously included in the software. The output of the DIRSIG model can then be rendered and viewed using various sensor configurations. Remote sensing information can then be gleaned from the rendered images.



## Improved Analytics for Dynamic 3D Security Systems

191160 | Year 1 of 2 | Principal Investigator: D. E. Small

### Project Purpose:

The current methodology for the design and implementation of physical security systems (PSS) is significantly outdated, and does not take into account the rapid advances in unmanned systems that can be used offensively or defensively. Two current tools are the Design and Evaluation Process Outline (DEPO) and the Estimate of Adversary Sequence Interruption (EASI). Both of these lack the ability to characterize dynamic sensors that move and 3D threats such as unmanned aircraft systems. The main question which this project hopes to answer is: how can we better adapt our mathematical models of physical security systems to modern security capabilities and threats provided by unmanned systems?

If the state of health of a PSS is visualized as a heat map, it would appear green around the perimeter when all the sensors are functional. If a sensor malfunctions, that area would turn into a dark red spot, indicating a vulnerability that might not be detected quickly. If the sensor is mobile, the hotspot is spread over a larger area with a lighter color of red, lowering the overall chance that the vulnerability could be exploited.

This project will derive new spatiotemporal models for the probability of detection for PSS that work with dynamic 3D sensors and threats. This work will positively impact our ability to model a modern PSS with mobile sensors and actuation. The technical approach this work will take will be to develop new models that address the shortcomings of DEPO/EASI allowing for new detection technologies such as pan/tilt/zoom cameras and unmanned systems. The team will research new algorithms that use principles of pursuit-evasion in the solution space of art gallery approaches with flexible optimality constraints. Lastly, this effort will develop a computational approach to testing and evaluation of physical security system designs. Theoretical models will be tested using modeling and simulation techniques.

## Improving Render Safe Capabilities for National Security from Chemical and Biological Dissemination Devices

191151 | Year 1 of 3 | Principal Investigator: A. L. Sanchez

### Project Purpose:

Chemical and biological (C/B) threats represent an increased vulnerability to national security, which could affect both military and civilian populations. In large scale settings such as major metropolitan areas, these C/B threats can be deployed in various forms, including sophisticated deliberate dissemination of C/B agents using liquid or powder dispersal devices. Such events can profoundly and disproportionately impact public health, infrastructure, and the economy. Unfortunately, such devices have not been well characterized, and can have large technical differences in effectiveness due to variations in state and non-state actor expertise and available resources. These differences introduce large uncertainties in plume modeling and make render-safe techniques ineffective and potentially unsafe.

Consequently, it is critical to better understand how such devices might work and establish an empirical database in order to characterize source terms, develop appropriate render-safe techniques, and explore potential failure modes. This project intends to develop novel methods for characterizing C/B devices that will allow significant improvements to both aerosol dispersion modeling of C/B events and render-safe technologies, protocols, and procedures. This research will significantly improve our understanding of dissemination efficiency, agglomeration and de-agglomeration physics, and the particle size distribution as a function of aerosol dissemination device design alternatives which are presently poorly understood.

By developing experimental parameters to better characterize unverified source terms, this work will reduce uncertainties in modeling inputs; thereby enabling more accurate predictions for decision makers, decreased response time for first responders, and improved situational awareness for consequence management. Source terms will be characterized according to traditional aerosol physics (e.g., particle size, concentration, release, and dispersion efficiency), which have not previously been thoroughly evaluated. This will provide valuable information for plume modeling approaches that continue to use highly idealized, and often criticized, instantaneous point release parameters as the current standard.



## Instrumentation Infrastructure for Cyber Emulations

191165 | Year 1 of 2 | Principal Investigator: V. Urias

### Project Purpose:

Sandia developed the Emulytics™ analysis to deploy cyber experiments at various levels of fidelity in a rapid and reliable manner. This experimental approach affords the analyst a controlled environment that can be used to model real world systems. It also provides the ability for extensive instrumentation to gather data from nearly all components deployed in the system. These platforms are built to answer questions; however, to date, the sophistication of the question has been focused on gross level impacts (e.g., counting packets, sessions, transactions, number of hosts, etc.). The ability to measure cyber effectiveness is predicated on the assumption that the operators, users, and others have prior and complete understanding of the effects and impacts caused by cyber adversaries.

Obviously, this is often not the case. When compared to the physical world, cyber is quite different in that it does not follow physical scientific laws; rather, cyber is unbounded because it is human-made. As a result, understanding and quantifying effects are still an immature science. In order to develop a foundation for identifying and bounding the issues, Sandia is approaching the problem empirically through experimentation.

In order to provide empirical results, there is an exigent need to develop better data gathering (i.e., instrumentation) understanding and techniques to ingest the data. This project will advance cyber analysis platform modeling technology and provide a novel capability for the analysis of cyber impacts on networks.

## Magnetic Smart Tags (MaST) for Arms Control and Treaty Verification

180893 | Year 2 of 2 | Principal Investigator: E. Langlois

### Project Purpose:

The ability to track nuclear material is critical to nonproliferation. Radio frequency (RF) tags are frequently used in national security applications, but sometimes cannot be used for technological, operational, or safety reasons. Magnetoelastic tags are an alternative technology and are a familiar security measure used in stores to prevent theft. Current magnetoelastic tags are large, single frequency devices, cut from strips of an amorphous magnetic material. They only convey information that a tag is magnetically activated (e.g., when passing through a portal) limiting their utility. A more useful tag would be small, cheap, and respond with a unique combination of multiple resonant frequencies and would also detect environmental parameters of interest such as variations in temperature, pressure, and pH.

In this project, we developed novel, wireless, passive, physically unclonable magnetic smart tags for tracking nuclear materials and treaty monitored items. Recently, giant magnetostriction has been observed in CoFe thin films fabricated by sputter deposition, a technique often used in microfabrication. Unfortunately, sputter deposited materials suffer from a high degree of intrinsic stress, slow deposition rates, and lack compatible anisotropic patterning etch processes. We created magnetoelastic smart tags (MaSTs) by electrochemical deposition (ECD), a cost-effective, batch manufacturing process, and demonstrated a first-of-its-kind electrodeposited CoFe film with a saturation magnetostriction ( $\lambda_s$ ) value of 78 ppm. The ECD process enabled released, free standing resonators with minimal stress gradients. Finally, a first-of-its-kind microelectromechanical system (MEMS)-based capacitive magnetostriction test structure was developed for both magnetostriction characterization and RF MEMS applications.

The MaSTs are multifrequency tags capable of providing millions of possible codes for tag identification. They may be safely interrogated near high explosives and through barriers, where RF tags cannot be used. They would be especially suitable for national security missions where radiation hardness, tamper resistance, immunity to long-range interrogation by adversaries, zero power (passive), and code complexity are important.



## Modeling Metal/Metal Compound Combustion for Energetic Material Enhancement

191176 | Year 1 of 2 | Principal Investigator: D. J. Allen

### Project Purpose:

The purpose of this project is to understand metal combustion through modeling and experimental validation. The goal of the research is to include the energetic contribution of burning metal particles within simulations such that the energetic performance of devices can be predicted when specific metal additives are used. Metals are commonly added (primarily in powder form) to increase the energetic output of devices such as explosives, shape charges, propellants, etc. Metals have a high energy density but are relatively difficult to ignite and are slow to react, which adds varying time scale complexity to the systems of interest.

Currently, it is experimentally known that the addition of metal particles will increase the over-pressure of energetic systems in certain applications; however, there is little predictive capability of performance due to many factors. First, for many metals, the combustion mechanism is not well understood. Second, for those metals where the combustion mechanism is well understood (aluminum, magnesium), it is difficult to incorporate metal combustion into dynamic calculations where the time scale of combustion tends to occur over a longer period than the shock physics.

There is a fundamental understanding for how common metal particles burn that exists in the literature, especially for aluminum particle combustion down to the micron scale. The ability to include these mechanisms within a fluid dynamics simulation code would significantly improve the ability of users to predict energetic output in specific applications and greatly enhance the ability to tailor a device to an application.

The key hurdle will be the implementation of the particle combustion model into a simulation and validating this model. The proposed work is innovative and different from other attempts in that it combines shock and hydrodynamic effects of high explosives making this a high risk, potentially high reward research endeavor.

## Online Mapping and Forecasting of Epidemics using Open-Source Indicators

173112 | Year 3 of 3 | Principal Investigator: J. Ray

### Project Purpose:

We propose to develop a data assimilation (DA) system that combines open source indicators (OSI) of disease activity, as well as meteorology to track and forecast disease outbreaks. Fast, dependable forecasting of disease activity can revolutionize medical and/or biodefense planning and response, but the long delays in collecting public health data, and inadequate spatial coverage means such data is of limited use.

Online OSI of disease activity (e.g., disease-related searches, media reports, etc.) and meteorology are strong covariates of outbreaks. They are readily available, timely, and have far superior spatiotemporal resolution than public health data, especially in developing countries. Currently there are no DA methods that can fuse them to compensate for delayed/unavailable public health data, nor meteorology-driven disease models for accurate forecasting. We propose to develop the methods and models and integrate them into a DA framework.

Our key hypothesis is that OSI and meteorological data are sufficiently rich to construct a spatial model of disease activity. Within the DA framework, the spatial model will interpolate sparse disease data using information gathered at monitored sites (generally large cities). Scalable ensemble Kalman filters will provide the mathematical underpinnings of data fusion so that the framework can be applied to country-sized problems.

The potential of DA has not been applied to disease forecasting because it has relied on sparse public health data. OSI and our DA framework would be a novel development with impact in data-poor regions. We will demonstrate this by tracking the evolution of the annual dengue outbreak in India using OSI data from HealthMap.





## Polarimetry for Extended Persistence and Range in Fog for Infrastructure Protection

191184 | Year 1 of 3 | Principal Investigator: D. Scrymgeour

### Project Purpose:

Many national security and infrastructure protection missions have a critical need to image in fog and obscuring environments (dust, oil plumes, underwater), and any potential gains can significantly improve the performance of perimeter-based physical security. Previous work by Sandia and others has demonstrated in both simulation and experiments that using circularly polarized light has clear advantages over linear and unpolarized light for signal propagation/range enhancement in fog and dust in visible, mid-wave, and long-wave infrared spectra. These exciting results, however, need to be carried forward into realistic fog conditions and offer a ripe area of fundamental research.

The goal of this research is to demonstrate that tailored wavelength and polarization selection can provide substantially increased performance in foggy conditions compared to traditional intensity-based techniques. This will involve designing, building, and validating new experimental setups at different wavelengths in the Sandia fog tunnels, which are capable of creating and sustaining controlled fog that can simulate specific fog conditions. We will focus on developing measurements and metrics used to validate the experiments in the simulated fog environments. These experiments will be used to validate our simulation tools that will be similarly expanded to investigate different wavebands and fog distributions. This simulation tool can then be used to explore different environments to optimize signal persistence in environments with critical national security importance.

Proving the utility of polarization requires basic research and development to achieve a body of knowledge that will inform future solutions in a range of diverse scattering environments. The systematic and fundamental study of the persistence of polarized light in fog environments will leverage Sandia's unique fog simulation facility.

## Rapid Automated Pathogen Identification by Enhanced Ribotyping (RAPIER)

191175 | Year 1 of 3 | Principal Investigator: M. Bartsch

### Project Purpose:

As illustrated by the recent Ebola crisis, effective response to an infectious disease outbreak (natural or man-made) requires local diagnostic infrastructure that responds rapidly with sufficient throughput. Countering global emergence of new viruses and pan-/multidrug resistant bacteria, a White House, Defense Threat Reduction Agency, and Center for Disease Control top priority, also requires new approaches that are low cost and low resource but have high technical flexibility. Molecular probe-based or traditional culture diagnostics are limited in target range by available reagents requiring laboratory infrastructure and time-consuming steps. Translating these methods into a universal diagnostic platform for use in a resource-limited setting has proven virtually impossible, necessitating a dramatically different approach.

We propose to create a universal bacterial pathogen identification and characterization tool based on nanopore DNA sequencing. Our approach leverages the revolutionary Oxford MinION nanopore sequencer, which is a palm-sized, laptop-powered, solid-state device that passes DNA through synthetic biofunctionalized pore structures. After library preparation, the MinION produces long (>5 kilobases (KB)) DNA sequence reads in real-time, but with poor nucleotide base calling accuracy (~65%). We hypothesize that: 1) microfluidic library preparation enables rapid, amplification-free DNA library preparation for MinION sequencing from small starting amounts, 2) targeted sequencing of DNA regions (e.g., entire ribosomal DNA or rDNA operon) containing both conserved (near-universal) and hypervariable (highly distinctive) regions will allow universal bacterial strain identification, and 3) despite sequencing errors, the structural repeats combined with the long reads will allow highly accurate, strain-specific nanopore sequence genotyping, or "nanotyping" of bacterial pathogens.

We propose to leverage fundamental microfluidics and nanoscale phenomena with advanced molecular biology methods to characterize genetic information at the single molecule level. A prototype microfluidic front-end automating the key elements of the nanopore sequencing sample preparation workflow will be developed, significantly integrating and demonstrating the critical operations derived from proof-of-concept experiments in a format suitable for laboratory proof-of-principle testing.



## Real-Time, Autonomous Field Surveillance for Vector-Borne Pathogens

173111 | Year 3 of 3 | Principal Investigator: R. Meagher

### Project Purpose:

Vector-borne pathogens including arboviruses such as Dengue Virus and Rift Valley Fever Virus, as well as parasites such as Plasmodium are among the most significant emerging (and re-emerging) pathogens worldwide. The recent spread of West Nile Virus to the western hemisphere provides a striking example of how quickly a vector-borne disease can spread across borders and oceans and become endemic across entire continents within a few years. Vector-borne diseases represent an acute threat to military personnel stationed overseas, particularly in tropical regions, and they are also potential agents of bioterrorism, directed either against humans or livestock. Conventional vector surveillance is a low-throughput process dependent upon skilled labor and detailed laboratory analysis. Novel approaches are required to improve the spatial and temporal resolution of vector-borne disease surveillance to better combat the spread of vector-borne viral diseases.

We propose to develop and deploy a new generation of rugged yet inexpensive “smart traps” to perform autonomous field surveillance of vector-borne pathogens, with daily assays and wireless data reporting. Our approach represents a revolutionary advance in vector surveillance, which presently relies upon skilled labor and minimal technology for data collection. Long-term, our smart traps will reduce costs by reducing the labor bottleneck in vector surveillance; but to encourage adoption in the short term, the smart traps must be simple, reliable, accurate, and inexpensive to deploy. Creating a reliable, accurate device within these constraints requires creative new approaches to engineering autonomous systems, emphasizing simplicity of design in place of costly, complex components.

This project aims to develop a fundamentally new technology for vector-borne disease surveillance and pursues advanced detection and assay technologies that are currently at a low technology readiness level (TRL) and high risk. The effort builds upon Sandia’s expertise in systems engineering and will establish a unique, novel capability for environmental monitoring to address needs in biodefense and emerging infectious disease surveillance.

## Risk Evaluation for Identification and Intervention in Dual Use Research of Concern for International Biological R&D Activity

192787 | Year 1 of 1 | Principal Investigator: K. A. Jones

### Project Purpose:

This project sought to develop a mathematical optimization framework for assessing and mitigating risks associated with dual use research of concern (DURC). Dual-use biotechnologies can be used both legitimately for the public good and maliciously for bioterrorism, and hence, pose a major national security threat. Despite the potential for dangerous worldwide impacts, the scientific community has not yet identified a rigorous method for minimizing bioterrorism or biosafety risk without hindering the progress of biotechnology research intended to protect public safety. The goals of the project were to: 1) provide a defensible approach for incorporating a mix of qualitative and quantitative subject matter expert assessments of risk and 2) support identification of optimal risk mitigation strategies that consider tradeoffs between benefits and multiple dimensions of risk. Previous research has made progress toward developing methods of both biosafety and biosecurity risk assessment (i.e., producing the data required to conduct risk-benefit analysis) and US government policies for DURC and the National Science Advisory Board for Biosecurity (NSABB) deliberative process for gain of function research produced a conceptual approach and set of principles to guide funding decisions (i.e., producing the parameters required for prioritization of benefits and risks). Yet, a gap remained in bringing together these developments in a comprehensive decision analysis framework that integrates risk evaluation and mitigation. This research focused on filling that gap via a portfolio level risk mitigation mathematical model.

An NSABB report illustrated that agencies have the most control at the research proposal and funding stage, and thus our research focused on mitigating risk and exploring risk tradeoffs at this stage.



## Sampling-Based Algorithms for Estimating Structure in Big Data

186366 | Year 2 of 3 | Principal Investigator: K. M. Matulef

### Project Purpose:

The purpose of this project is to develop sampling-based algorithms to discover hidden structure in massive data sets. Inferring structure in large data sets has become an increasingly common task in many critical national security applications, such as cybersecurity and remote sensing. These data sets come from many sources, such as network traffic, sensor data, and data generated by large-scale simulations.

Identifying hidden structure in this data is crucial to exploiting it effectively, but the data is often so large that traditional data mining techniques are time consuming or even infeasible. To address this problem, we focus on algorithms that do not compute an exact answer, but instead use sampling to compute an approximate answer using fewer resources. In particular, we look at a class of algorithms called streaming algorithms that are designed to handle high throughput streams of data using only a small amount of storage space—a fraction of the length of the stream—while producing provably good approximations.

One of the quantities of interest that we examine is the degree distribution of a graph (i.e., the distribution of the number of connections for each node in a network). The degree distribution is a fundamental graph property, but for massive networks consisting of a long stream of edges, computing it exactly in real-time is not feasible. We consider a variant where we need only produce an approximation. Previous work has only considered this problem for special cases. We improve upon prior work by augmenting it to handle streams with repeated edges, and structures that evolve over time, making our algorithm suitable for real-world streams. We also develop streaming algorithms for common tasks such as finding highly similar items in a stream, and weighted sampling of items with dynamically changing weights. We expect these to serve as building blocks for other types of estimations on streaming data.

## Single-Volume Neutron Scatter Camera for High-Efficiency Neutron Imaging and Source Characterization

173113 | Year 3 of 3 | Principal Investigator: E. Brubaker

### Project Purpose:

The neutron scatter camera (NSC), an imaging spectrometer for fission energy neutrons, is an established and proven detector for nuclear security applications such as weak source detection of special nuclear material (SNM), arms control treaty verification, and emergency response. Relative to competing technologies such as coded aperture imaging, time-encoded imaging, neutron time projection chamber, and various thermal neutron imagers, the NSC provides excellent event-by-event directional information for signal/background discrimination, reasonable imaging resolution, and good energy resolution. Its primary drawback is very low detection efficiency due to the requirement for neutron elastic scatters in two detector cells. We are developing a single-volume double-scatter neutron imager, in which both neutron scatters can occur in the same large active volume. If successful, the efficiency will be dramatically increased over the current NSC cell-based geometry. If the detection efficiency approaches that of coded aperture imaging, for example, the other inherent advantages of double-scatter imaging would make it the most attractive fast neutron detector for a wide range of security applications.

There are significant technical challenges to implementing this concept, especially when resolving nearby scatter events, which we believe can be resolved using recent advances in photodetection technology and associated electronics. If we are successful, a calculation of the achievable improvement in effective area is at least an order of magnitude. The detector footprint will also be greatly reduced.

This is a high-risk, high-payoff detector R&D project. The key hurdle is the difficulty of resolving two proton recoils in a single scintillator volume at spatial and temporal separations of order 1 cm and 1 ns, respectively, via the isotropically emitted scintillation light. We intend to demonstrate the ability to achieve this using state-of-the-art photodetectors and electronics.



## System Theoretic Framework for Mitigating Risk Complexity in the Nuclear Fuel Cycle

191154 | Year 1 of 2 | Principal Investigator: A. D. Williams

### Project Purpose:

This project aims to create a systems-based methodology to manage the complex risks of the nuclear fuel cycle (NFC), given how the increasing global demand for electricity and climate change concerns have expanded the NFC infrastructure that could potentially be exploited. This expanding NFC infrastructure combined with a multifaceted threat environment presents increasingly complex security risks—a risk space captured in the safety, security, and safeguards (3S) challenges of transporting spent nuclear fuel (SNF). For example, the expected US shipments of SNF in 2055 and the emergence of multimodal nuclear fuel transportation routes for new nuclear energy programs illustrate how quickly SNF-related risks increase in complexity. In addition, current SNF transportation analyses heavily emphasize safety, lightly touch security, and typically ignore safeguards. The S&T question that motivated this research relates to suggestion that certain elements of safety, security, or safeguards technologies (e.g., cameras) could be ‘shared’ as an expected benefit of integrated 3S approaches.

Specifically, developing a 3S system framework is expected to identify gaps, interactions, and conflicts that would be missed by the traditional approach of analyzing each 3S subsystem in isolation. While there have been a number of conceptual efforts on integrated 3S approaches, there has not been any serious research regarding systems analysis or modeling of the 3S system. This work will adapt two novel analytical approaches—dynamic probabilistic risk analysis (DPRA) and system-theoretic process analysis (STPA)—into an implementable framework pushing the cutting edge of 3S research beyond conceptual efforts. Traditional SNF transportation evaluation methods for 3S are challenged by ignoring interdependencies and assuming time independent domain risk mitigation strategies. In contrast, our research utilizes system-theoretic approaches and dynamic risk assessment frameworks to assess, manage, mitigate, and reduce complex risks of SNF transportation with a time dependent, dynamic control theoretic complex system model.

## Understanding Chemical Threat Agent Interaction with Concrete: Critical Step Toward CI Restoration

180896 | Year 2 of 2 | Principal Investigator: C. M. Tenney

### Project Purpose:

Restoration of critical infrastructure (CI) after attack with a “persistent” chemical warfare agent (CWA) is not guaranteed. With very low vapor pressure, high chemical stability, and extreme toxicity, persistent CWAs are designed to cause social, economic, and mission disruption through long-term access denial. A lack of understanding of the transport and fate of persistent CWA threats hinders the development of safe and cost-effective remediation and recovery strategies. Of particular concern is the transport and fate of persistent CWA in concrete, a ubiquitous infrastructure building material that is costly to remove and replace.

We developed atomistic models for relevant CWA molecules—multiple mineral surfaces, including the primary calcium-silicate-hydrate (CSH) phase of cement; and molecular species representative of decontamination material ingredients. Using these atomistic models, both first-principles and classical molecular dynamics simulations were conducted to study CWA fate and transport in systems composed of hydrated mineral surfaces.

First-principles molecular dynamics simulations were used to investigate the dissociation of sarin on the CSH mineral tobermorite, a surrogate for the primary mineral phase present in portland cement. Results indicate that both adsorption site and humidity of the local environment significantly affect the sarin dissociation energy.

Classical molecular dynamics simulations were used to investigate and quantitatively predict the partitioning and sorption of CWA molecules on mineral surfaces in the presence of water and analogue decon fluid molecules. These results clarify mechanisms by which mineral surfaces, water, and decon molecules can affect CWA availability and persistence.

These simulation capabilities provide a valuable tool for the development of more efficient and effective strategies for remediation and clearance of infrastructure following the release of a persistent CWA. The tools and techniques developed in this project can also be applied to other problems involving species partitioning in multiphase systems, for example more efficient recovery of hydrocarbon energy sources.



## Using Data Science to Improve Theorems of Human Performance in National Security Domains

191166 | Year 1 of 2 | Principal Investigator: D. J. Stracuzzi

### Project Purpose:

We propose to modify existing predictive theories of visual search performance to better model expert performance, which can then be used to better engineer interfaces for data analysis platforms in national security missions. Our goal is to understand the nature and boundaries of expert visual search performance. Existing theories are based on novices performing general tasks, yet recent Sandia research shows that novice performance differs substantially from experts in specialized, high-consequence domains.

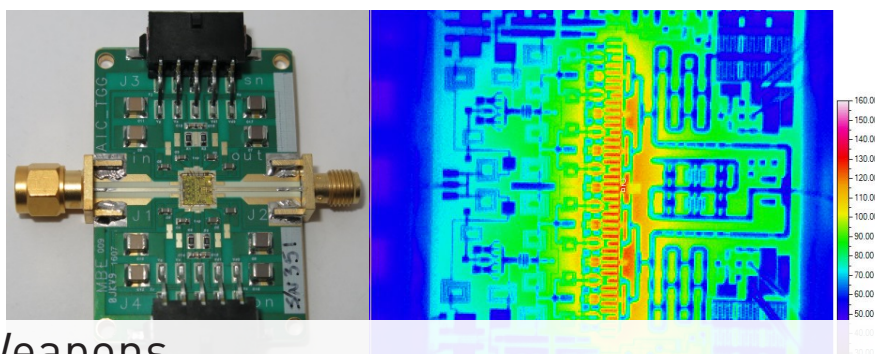
Visual search considers the perceptual problem of actively scanning a complex scene to locate target objects. DOE-relevant examples arise in nuclear nonproliferation activities that rely on specific patterns in massive data stores. We take a hard-science approach to extending existing theory. We will develop new data science-based analysis methods for extracting patterns and techniques from visual search data. We will then update existing theory to account for the expert data, including developing hypotheses that will allow us to test the revised theory. This work focuses on how humans interrogate data, and complements other projects seeking to automate that interrogation.

Developing the insights needed to broadly support Sandia's national security missions requires development of data analysis tools and theories that generalize across multiple domains. This project investigates the impact of key properties of national security domains on analyst performance that have not received attention in the academic literature. These properties include high-consequence outcomes, time pressure, and adversarial obfuscation efforts.





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# Nuclear Weapons

The primary goal of the Nuclear Weapons (NW) Investment Area is to support advancement of the NW Mission Area Strategy through investments in leading-edge science and the incubation of new technologies and capabilities. These investments are intended to promote innovation in our core products to meet future mission needs and to develop new tools and technologies for design, qualification and surveillance with an overarching goal of improving cost effectiveness, agility, and assurance throughout the life cycle.

The figure above shows: (left) 60 Watt power amplifier prototype package; (right) infrared image of the power amplifier package demonstrating thermal robustness. (Project 173187, Reconfigurable Matching Networks for High-Efficiency GaN Power Amplifiers)

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## Additive Manufacturing of Metallic Components by Laser Powder Forming

181204 | Year 2 of 3 | Principal Investigator: C. W. San Marchi

### Project Purpose:

Additive manufacturing (AM) technologies offer a new platform for innovation of advanced components. Reasonably complex geometrical features can be manufactured by laser powder forming, which has demonstrated the potential to enable innovative designs, reduce costs, and lower manufacturing energy consumption. The engineering community, however, lacks confidence in the structural integrity and reproducibility of additively manufactured metals, in particular the distribution of defects (e.g., interfaces and porosity) and presence of residual stresses. In short, the lack of a robust understanding of the physical and mechanical metallurgy of AM materials and the lack of predictive manufacturing simulation tools are two important limitations of broad acceptance of AM by the design community. We propose a metallurgical investigation, in collaboration with the University of California-Davis, to provide a framework for understanding microstructure, fracture properties and residual stress in AM structures. The three objectives of this effort are: 1) to benchmark the microstructure and structural properties against known properties of nominally equivalent stainless steels, 2) to assess the defects intrinsic in AM and the sensitivity of the AM microstructures to process variability, and 3) to optimize the AM process for combination of strength and fracture resistance (defect tolerant design metric), including control of residual stress. This experimental study will also interface with complementary modeling efforts. The outcome of this investment will be a significant advance toward providing a design basis for defect tolerant design of AM components as an alternative to conventional materials and manufacturing.

## Additive Manufacturing of Porous Materials

180929 | Year 2 of 3 | Principal Investigator: D. Robinson

### Project Purpose:

Additive manufacturing is heralded by mechanical engineers as a new path to load-bearing structures that use material very efficiently. The emerging field also has promise in chemical engineering, where there is ubiquitous reliance on randomly packed powders in chemical reactors; electrodes and separator membranes for batteries and fuel cells; separation columns, filters, and other devices that manipulate fluid flow and ion transport. In cases where randomly arranged materials have been replaced by deterministically fabricated devices with optimized geometries, major performance and efficiency improvements have been achieved. Notable examples can be found in gas chromatography, microfluidic medical devices, and recently emerging “3D battery” structures. However, such improvements are not widespread because the appropriate fabrication techniques are not available in most situations.

The key technology gaps are:

- Limited access of additive manufacturing techniques to the 1-100  $\mu\text{m}$  length scale, especially for inorganic materials. This length scale is often needed for efficient fluid-solid contact.
- Lack of parallelism in existing fabrication methods, which typically involve a rastered laser or extruder.

The goal of this project is to develop efficient, scalable manufacturing methods for porous chemical engineering devices, relying on several key Sandia technologies:

- Nanoporous powders of well-defined particle and pore size that can be sintered through mild chemical or thermal treatments
- Photochemical and electrochemical methods that permit deposition a plane at a time, without relying on rastering
- Small-scale platforms for high-throughput characterization of filters and separation columns
- State-of-the-art powder-based 3D printers for inorganic materials

We will focus on delivering, as a proof of principle, a sub-millimole scale separation column that achieves much more sharply defined separations at a much lower pressure drop than a similarly sized packed-powder column.



## Additively Manufactured Shock Absorbing Engineered Materials

193407 | Year 1 of 3 | Principal Investigator: N. Leathe

### Project Purpose:

There is a need for advanced shock absorbing materials for increased performance in many Sandia applications. Additive manufacturing offers significant advantages in the development of shock absorbing material as it increases product development agility and design freedom. Shock absorption could envelop an entire product or only shock-critical components. This project will develop an innovative, additively manufactured, shock absorption honeycomb material that can provide fully recoverable isolation from moderate impacts to protect underlying components with designed thresholds for transmitted acceleration, while transmitting higher impact loads to potentially activate those components, and distinguishing between these loads entirely passively via structural mechanisms. The University of Texas at Austin has previously demonstrated a plastic additively manufactured shock absorbing honeycomb material. This material was shown to reduce the peak response force of a dropped object by 1/20th with fully recoverable, elastic absorption mechanisms. However, Sandia applications will need metallic versions of the material that can absorb impacts at magnitudes and speeds two orders of magnitude larger than those previously demonstrated by Texas researchers. Models of material performance will be expanded to capture high-speed impacts and additively manufactured metals. Absorption mechanism geometry will be designed to meet spatial and isolation targets as closely as possible. Model-based predictions will be validated with scaled experiments. Allowable tolerances will be investigated with model-based studies, combined with empirical data from additive manufacturing trials.

Current research with plastic shock absorbing materials must be extended to metallic materials for survival in extreme environments. A parametric approach to the characterization of the metallic behaviors and dependence on process parameters and production tolerances is needed for a complete understanding of the material. This understanding will ensure appropriate application for national security products and provide a comprehensive grasp on performance, variation, and predictability.

## Bridging the Gap: Evaluating Compatibility and Reliability of Interfaces between Additively Manufactured and Conventional GTS Components

191227 | Year 1 of 3 | Principal Investigator: K. Allen

### Project Purpose:

Currently, a paradigm shift away from the strict use of conventional manufacturing towards the incorporation of additive manufacturing (AM) for nuclear weapon (NW) components in the stockpile is being considered. While the use of AM is expected to enable increased affordability, agility, and assurance of components in the NW space, an effort to characterize and evaluate the interfaces between AM components and conventional components must first be performed. With regards to limited life component exchange (LLCE) components, such as gas transfer systems (GTS), AM parts stand to be interfaced with conventionally manufactured parts over varying timescales, driving the need for a fundamental understanding of the interaction of these two component types. The question is how will the inherent heterogeneities (microstructure, composition, porosity, and surface roughness) of AM parts affect their interfacing with GTS conventional components? This work seeks to characterize the dynamic interfaces formed between machined AM surfaces and conventional hardware following explosive valve actuation and resistance forge welding (RFW), two GTS processes with severe sliding contact environments. Various microstructural imaging techniques and profilometry will be used, and interfacial properties such as dynamic friction, galling resistance, and other tribological characteristics of these surfaces will be measured. Successful characterization of AM component surface microstructure and how this correlates with interfacial mechanical properties between these two component types will aid in providing confidence that the marriage of AM components and conventionally manufactured parts for GTS is achievable, incentivizing use of this efficient and cost-effective manufacturing technique in future product development cycles.

AM has garnered the interest of the Nuclear Security Enterprise (NSE) because of the possibility of producing quality parts quickly and affordably. However, little has been done to fundamentally characterize AM (net-/near-net shape condition) and conventional hardware interactions. This research aims to understand the interactions between AM and conventional parts and assess AM suitability for NW applications.



## Cognitive Data Science for Neutron Generator Predictive Pattern Analysis

173153 | Year 3 of 3 | Principal Investigator: S. H. King

### Project Purpose:

Recent neutron generator problems with high voltage breakdowns, and processing variation, have highlighted the need to increase understanding of neutron tube(NT) and neutron generator (NG) performance. Over 25 years of data from neutron generator testing are available for analysis—an underutilized resource that offers undiscovered information on behaviors, trends, and relationships. As we gain sophistication in collecting and modeling this information, it is critical that we support the development of leading-edge technologies to provide predictive assurance of product performance.

To address this challenge, our project focuses on the performance aspect of NTs and NGs where waveforms of data are collected for each tube and generator as performance assessments relative to requirements. Each of these waveforms contains thousands of data points. Human visual pattern recognition and interpretation are the primary methods to assess the waveforms. Trained, experienced personnel perform this “eyes-on” analysis. One primary research challenge was to assess whether expert visual pattern recognition on tester waveform images can be captured and integrated into automated models of product performance patterns (failure/success); and, together with models of the underlying data, provide leading indicators for future product performance.

Underlying multivariable relationships in NG/NT waveform data were modeled. In addition, expert visual pattern recognition of waveform images was successfully captured and integrated into the model. The dial-a-cluster algorithm gives analysts a broader view into data—increasing the scope of questions and answers that can be ascertained. User studies showed quick adaptability to the tool and this new mode of interaction with the large data sets.

Although this project focuses on NG and NT data, developing cognitively informed models of waveforms is a novel approach in product engineering analysis. This work will provide novel technologies to address design and performance issues proactively and enhance the quality of current and future designs.

## Compressed Sensing to Support Reduced Flight Testing

173180 | Year 3 of 3 | Principal Investigator: M. O. Pugh

### Project Purpose:

In telemetry there is a drive to quantify margins and uncertainties. This drive requires an increase in sensor data by an order of magnitude, yet there is no corresponding increase in the bandwidth. Furthermore, the reduced number of flight tests makes it imperative to maximize the amount of data collected per flight test. Traditional compression methods prove inadequate as they require an increase in onboard complexity, resulting in greater power consumption and volume. Complex onboard processing introduces latency, limiting the capability for end-event measurements. Using the same compression algorithm for various types of telemetry signals may not be possible. The cost and complexity of having multiple algorithms based on traditional compression schemes make this approach unfeasible.

Compressed sensing (CS) is a new, fast growing field that fundamentally changes data acquisition by allowing sampling at sub-Nyquist rates. Our research will provide insight on how to implement concepts of CS in telemetry systems. We seek to show that CS has comparable compression performance with traditional compression techniques, while offering significant decrease in cost, power, on-board processing, and complexity.

In our work, the CS-based algorithm would allow for a common compression algorithm for different types of telemetry signals. To the best of our knowledge, this is the first time that multiple different types of signals are being compressed using a CS-based approach. We intend to implement the proposed algorithm in hardware. This work will lay the foundation for developing sensors that inherently acquire signals in compressed form, making the compression step obsolete.





## Contactless Communications and Power Transfer Bridge

196604 | Year 1 of 1 | Principal Investigator: P. J. Robertson

### Project Purpose:

The next generation nuclear weapon (NW) system architectures intend to utilize hermetically sealed modules—an approach that will revolutionize weapon development by enabling flexible, adaptable, interchangeable and upgradeable systems, across multiple weapon platforms. The intent of this project was to develop technology capable of supplying power and data communications across a metal barrier. Multiphysics 3D simulation software was used to model the hardware and results were compared with laboratory measurements. Models enable predicted design performance of future applications. Two specific areas of research included iron nitride for improved magnetic core performance and spray-on materials compatible with the core materials.

## Creating Robust and Secure Free-Space Optical Systems for Information and Power Transmission in Confined Environments

191234 | Year 1 of 2 | Principal Investigator: P. C. Galambos

### Project Purpose:

Nuclear Weapons (NW) power and information connections are point-to-point, necessitating system redesign to accommodate component upgrades. Future qualification and surveillance of NW systems will rely on embedded sensors that monitor critical component functionality and state-of-health. In this way, the expense associated with random removal and disassembly of weapons from the stockpile can be avoided, while enhancing weapon surety. Optical communication lends itself well to this application.

Despite extensive research on fiber optic communications, there are significant unaddressed challenges for NW applications. Power must be supplied to sensors and other components and signals transmitted in both directions. Signals must be routed in confined and densely packed spaces, without adding wiring and connector complexity. Furthermore, the components must be radiation hard.

We propose a novel optical architecture with common power and information interfaces. This architecture enables modular change-out of components. Free-space optics reduces the number of connections, minimizes connector size and complexity, and removes cumbersome electrical wiring. The high-risk challenges include developing: 1) narrow-optical-bandpass, electrically conductive windows for optical power transmission and signal interrogation of embedded sensors, 2) electro-optical shutters to open/shut the windows and steer the optical beams, 3) free-space signal and power routing architectures, and 4) high-power and modulation bandwidth radiation hard optical components.

Success in this project will allow consideration of optical interconnect architectures for future system designs targeting more affordability, agility, and assurance.



## Defect Characterization for Material Assurance in Metal Additive Manufacturing

180928 | Year 2 of 3 | Principal Investigator: B. H. Jared

### Project Purpose:

Additive manufacturing (AM) offers unprecedented opportunities to design complex geometries and topologically optimized designs for performance gains inaccessible under conventional manufacturing constraints. AM also introduces the ability to generate engineered materials with microstructures and properties that are impossible via traditional synthesis techniques. However, to facilitate adoption in high consequence nuclear weapon (NW) applications, fundamental questions regarding the intrinsic reliability and repeatable performance of additive metals must be answered. Distinct from traditional subtractive processes, component geometry and material are formed concurrently in additive processes and preclude an a priori knowledge of material performance from feedstock properties. Of particular interest are powder bed fusion processes where a laser scans across successive layers of metal powder to fuse material and generate the desired part geometry. Characterizing, predicting and controlling material properties are currently difficult for powder bed processes since they involve complex melting and solidification interactions, and are implemented on equipment lacking process feedback. Consequently, material performance is currently unquantified and introduces unacceptable uncertainties. This project will reduce these uncertainties by exploring the additive formation of a precipitation strengthened stainless steel relevant to NW components. Characterization will identify the nature of critical defects, and quantify how additive-induced defects impact material properties and performance. We will explore three optimization pathways: metallurgical modification of the feedstock powder, adjustment of the additive process parameters, and modification of post-forming aging heat treatment.

## Direct Mechanical Ignition of Reactive Materials for Improved Safety and Performance

180926 | Year 2 of 3 | Principal Investigator: C. Yarrington

### Project Purpose:

Direct ignition of nonexplosive, reactive materials through shock or shear loading could improve performance and safety for nuclear weapons components. A working knowledge of mechanical ignition would allow for simpler component designs that reduce hazardous handling and manufacturing steps, as well as the associated costs. For example, directly initiating a percussive battery's heat source would simplify future design and manufacturing efforts by eliminating an explosive device and increase performance through reduced turn-on time. Safety components—like failsafes/weaklinks—or component improvements—like fusible contacts to mitigate chatter—could also be realized. Unfortunately, the knowledge to accurately describe the response of reactive materials to high-rate, mechanical loads is unavailable. Difficulties in separating material property effects and the complexity of the process have limited our current understanding.

The purpose of this project is to discover the mechanisms leading to ignition in reactive nanolaminates during dynamic mechanical loading. Sputter-deposited nanolaminates allow for precise control of material properties, so effects of material property changes can be studied individually. Ignition limits will be probed by varying stress wave strength, orientation, microstructure, and material properties. Testing will uniquely isolate relevant loading conditions including planar impact, mixed compression/shear, and high shear. The physicochemical alterations leading to ignition will be characterized experimentally and described with numerical models to aid future material selection and material design. It will be possible through these experimental and numerical studies, to engineer reactive materials with tailored mechanical ignition characteristics, allowing component-level integration of mechanically ignited reactive materials and realization of safety/performance improvements.



## Electro-Syntheses of Intermetallic Couples as Thin-Film Heat Sources for Advanced Thin-Film Thermal Batteries

173184 | Year 3 of 3 | Principal Investigator: C. A. Apblett

### Project Purpose:

We seek to develop low-cost, high-energy electroplated heat sources based on Ni-Al intermetallic formation that can be rapidly formed into shape for use in advanced thermal batteries and for fast brazing, joining, and energetic components. Current heat sources of this type use alternating nanostructured layers of reactive metals made by sputtering—a process requiring thousands of iterations, high capital investment, and expensive shaping to fabricate the heat sources.

We focused on developing a dispersion electroplating method to achieve the necessary nanostructure between the reactive couples of Al and Ni. Ni nanoparticles were included within an Al plating bath and incorporated into the electrodepositing film. However, the fundamental science that underpins this is quite complex. Because agitation is needed to keep the particles in suspension and continuous flow to the plating surface is necessary to deliver particles to the growing film, the effects of shear and flow on the electrochemical deposition needed to be developed, and this turns out to be a strong function of the shear rate. This dependence complicates getting the correct stoichiometry of Al to Ni for complete reaction, as changes in the Ni arrival rate (shear) affect plating rates due to changes in the diffusivity of the ionic liquid. The knowledge gained in working with ionic liquids for aluminum deposition provided a significant increase in performance for the chemistries, and allowed for high purity films to be developed.

Heat sources for thermal batteries are currently based on perchlorate chemistries, and the aging of these materials is well understood. Because of the unknowns involved in nanofilm and intermetallic aging, this technology will not be adopted into a battery until the aging characteristics are known. The knowledge gained in working with ionic liquids for aluminum deposition provided a significant increase in performance for the chemistries, and allowed for high purity films to be developed.

## Engineered Composite Materials Science and Technology for Next Generation Glass-to-Metal Seals

173186 | Year 3 of 3 | Principal Investigator: K. G. Ewsuk

### Project Purpose:

Steadily increasing demands on nonnuclear components in weapons systems have pushed critical properties like the strength of traditional glasses in glass-to-metal (GtM) seals to their limits, eliminating margins critical to predictable performance and reliability. Glass-ceramics (G-Cs) in GtM seals have improved tolerance to cracking/chipping, but at the expense of robust manufacturability, and with unresolved hermeticity issues attributable to poor interface bonding. Novel, interface-engineered, advanced composites comprised of two or more chemically compatible materials can take advantage of the desirable attributes of the constituent materials, while circumventing their deficiencies. Particle-filled glass composites (FGCs) can be developed as new sealing materials to make improved performance and reliability GtM seals. Although introducing new materials always presents significant risk, the need and potential for better performance and reliability warrants the investment. FGCs offer enhanced manufacturability, performance, and reliability by combining the processing robustness and thermodynamic stability of a glass, with the physical stability, design flexibility, and enhanced performance of a crystalline solid. FGCs also afford more robust processing and greater control of microstructure and properties compared to G-Cs. To enable the design, development, and manufacture of advanced FGCs, enabling materials and process characterization and modeling tools and technology will be developed in this project, including: 1) experimentally validated molecular modeling to understand and control glass chemistry-structure relations important to interface bonding and seal reliability and 2) composite property and process modeling to understand, control, and optimize FGC design, manufacturability, and performance. A primary goal of this study is to test, refine, and validate glass chemistry-structure and FGC property and process modeling by comparison to experiment, verifying the potential of these tools in the development of advanced new sealing materials and technology.



## Multi-Material Additive Manufacturing for Trusted Ceramic Packages with Embedded Capacitors

191232 | Year 1 of 3 | Principal Investigator: S. S. Mani

### Project Purpose:

This project will investigate a multimaterial packaging approach using additive manufacturing (AM) to integrate novel, conformal capacitors within miniaturized, high reliability, and high performance substrates. Recent advancements at Sandia in AM focus on solid state deposition (SSD) processes as an alternative to melting/fusion-based commercially available 3D printing technologies. The newly developed SSD techniques lend themselves well to the codevelopment of unique substrate and capacitor designs through the utilization of integrated polymers, ceramics, and metals within the same package design. With these mixed material architectures, many technical risks must be accounted for to achieve the coupled optimization of manufacturability, custom-tuned electrical performance, mechanical reliability, miniaturization, and thermal performance. Some of these risks include dielectric/conductor print quality, field enhancement for novel capacitor designs, thermal expansion matching, management of interfacial/surface energy for reliable adhesion, and optimization of printing parameters for low thermal input, conformably printed materials. By addressing these issues, we will enable a series of advancements to potential applications such as neutron generators, fusing radar, firesets, and remote sensing. Potential advancements to these areas include higher voltage capacitors and capacitor miniaturization which leads to system miniaturization, decreased electrical loss, and enhanced system functionality.

AM using multiple materials provides significant innovation opportunities for microsystems. AM technologies provide the ability to create novel structures and apply materials in an atypical fashion onto traditional and nontraditional surfaces. This project will focus on the application of AM to create novel, multimaterial devices that take advantage of the capability offered through AM materials and technologies.

## Non-Linear Transmission Line Based Technology

173182 | Year 3 of 3 | Principal Investigator: J. M. Elizondo-Decanini

### Project Purpose:

The fundamental question of this project was: can we replace linear capacitors, used in a linear circuit, with nonlinear capacitors or even np-junctions in novel nonlinear circuit topologies? Is it possible to produce high voltage amplification to the point that we may replace conventional power supply technology, or increase efficiency beyond present legacy technology? We proposed to understand and develop nonlinear transmission lines, specifically to produce voltage pulse compression and amplification, for applications where high voltage (kV range) short pulse ( $\mu$ sec range) is needed for activities in Sandia's mission space and beyond. Theoretical and experimental research was performed to understand soliton production based on two different approaches: 1) nonlinear ceramics and 2) semiconductor np-junctions used in reversed voltage mode. We were able to master the science/technology of producing electrical solitons using a variety of configurations, and demonstrated replacement of ceramic capacitors with solid state np-junctions in compact kV range applications. We also developed a high impedance detonator capable of operation with solitonic high voltage pulses produced by nonlinear transmission lines, operated at low voltage inputs.

The project's original success measure was to multiply the input voltage to at least a factor of 3X with a stretch goal of 5X. The end result is that we demonstrated a multiplication factor in excess of 8X, with output voltages in excess of 100 kV.



## Optical Bus Architecture for VCSEL Transceivers

196470 | Year 1 of 1 | Principal Investigator: D. K. Serkland

### Project Purpose:

The question that inspired this research was: can an optical data bus be made that mimics the performance of a multidrop linear electrical bus? Traditional fiber optic data communication transceivers using vertical-cavity surface-emitting lasers (VCSELs) are designed only for point-to-point interconnects between two nodes. In contrast, multidrop electrical buses, such as the controller area network (CAN) bus, are designed to take advantage of the ability of several transistors to share a common electrical line in a wired or-gate configuration so that many nodes can communicate on a single electrical line. We proposed to develop a new optical bus architecture that used VCSELs and photodiodes to achieve the same functionality as the electrical wired or-gate, thereby allowing an optical implementation of a multidrop linear bus.

## Organic Semiconducting Materials for Thin-Film Optoelectronic Devices

173183 | Year 3 of 3 | Principal Investigator: K. Leong-Hau

### Project Purpose:

Detection of near infrared (IR) light with flexible, easily produced, and low powered devices is currently not possible. Limitations include high dark currents and manufacturing costs and low detectivities. These challenges led us to investigate semiconducting polymers as the active material for photodetectors and other optoelectronic devices. Our strategy to achieve the goal for fabricating near IR optoelectronic devices combines computational and synthetic chemistry with device fabrication and testing. This collaboration facilitates an iterative process to optimize parameters controlling important factors such as electron/hole mobility, optical band gap, and film morphology. Specifically, making polymers with a narrow band gap poses a synthetic challenge due to difficult monomer syntheses, high purity requires, and appropriate polymer structure. Challenging to computational chemists is developing a model or understanding of the factors controlling charge transfer from a p- to n-type material with the correct band offset. Characterizing these processes in devices, and fabricating prototypes that meet our systems' requirements is the last main challenge we seek to surmount. The greatest theoretic risk we face is that a suitable acceptor is not available for band alignment with our narrow polymer donor. A technical risk we face is that our synthetic chemistry takes longer than anticipated, limiting the scope and impact of the project. The fundamental nature of this R&D means that any advancements or discoveries will contribute to the larger scientific community.

## Radiation Hardness of MEMS Capacitive Accelerometers

173154 | Year 3 of 3 | Principal Investigator: B. D. Homeijer

### Project Purpose:

Fuzing options based on path length traveled are central to the performance of the ballistic legs of the nuclear deterrent. The approach of this project has been driven by the lack of available sensors that can meet the radiation hardness requirements. While evaluations of radiation effects on some commercial microelectromechanical systems (MEMS) accelerometers have been published, the fundamental understanding of why such devices fail in radiation environments is incomplete, and techniques for designing inherently hardened sensors based on this understanding have not been developed. Acquiring this knowledge is a necessary step to enable the development of an intrinsically radiation-hardened, large dynamic range accelerometer. The commercial MEMS inertial sensing market has not addressed this problem because the market size for radiation-hardened accelerometers is miniscule relative to consumer grade devices.

We proposed to investigate the fundamental effects of radiation on MEMS materials, including the physical mechanisms of radiation-induced dielectric charging and stiffness changes due to displacement damage. We then developed a modeling capability to quantify and predict changes in performance of MEMS-based electrostatic sensors due to these radiation effects. This combined knowledge allowed us to develop designs and processes that enable intrinsically radiation-hardened MEMS accelerometers and gyroscopes.

In the final year of the project, the materials and design efforts were combined and yielded a radiation tolerant accelerometer. This work has the potential to significantly improve sensing capabilities in nuclear weapons and space based applications by providing a previously unavailable radiation-hardened MEMS inertial sensing technology.





## Reconfigurable Matching Networks for High-Efficiency GaN Power Amplifiers

173187 | Year 3 of 3 | Principal Investigator: M. M. Elsbury

### Project Purpose:

Modern radar transmitters under development are based on single-chip gallium arsenide power amplifiers (PAs) capable of producing unprecedented levels of radio frequency (RF) power and integration. Unfortunately, because these PAs are designed to cover wide bandwidths, they operate with low power-added-efficiency (PAE), resulting in tremendous wasted heat. The thermal management problem created by this high power dissipation is a daunting technical challenge.

Gallium nitride is the next-generation RF semiconductor technology capable of operating at much higher voltages and temperatures than conventional GaAs. Recently, researchers have exploited the high voltage capability of GaN to design highly efficient, switching-mode RF PAs. Unfortunately, the maximum practical bandwidth of these switching mode PAs is too low for many applications.

This project investigated GaN custom radio frequency integrated circuit (RFIC) design for pulse-Doppler applications. In FY2014, efforts focused on the creation of a suite of fixed-tuning medium-power high efficiency GaN amplifiers. In FY2015 the focus shifted to creating a high-efficiency amplifier suite with increased output power and adding output tuning configurability. Finally, in FY2016, the project culminated in the creation of a high-power, high-efficiency suite of amplifiers incorporating output-power reconfigurability based on radar mission needs and integrating these PAs into high-reliability packaging solutions appropriate for future national security applications.

## Recycling Scandium and Erbium from Nuclear Weapon Manufacturing Operations

173156 | Year 3 of 3 | Principal Investigator: R. F. Hess

### Project Purpose:

The main goal of this project was to establish a scientific basis for the dissolution and deposition of lanthanides using ionic liquids (ILs). Initial efforts focused on isolating scandium metal from process-generated coated tungsten (Sc-W) crucibles as a benchmark. The separation of  $\text{Sc}^{3+}$  from other metal ions using solvent extraction techniques has been demonstrated but relies heavily on the use of concentrated acid and organic solvents similar to the PUREX process for actinides. In contrast, the IL dissolution of lanthanides has been relatively unexplored. ILs have low vapor pressures and larger electrochemical windows that will allow for the reduction of  $\text{Sc}^{3+}/\text{Er}^{3+}$ . Our approach was to develop tailored IL materials to selectively electrochemically dissolve scandium metal from the crucible and determine the conditions necessary to electroplate scandium metal. This novel IL solution route will also enable the more delicate instrumentation to be 'washed.' After the scandium is solubilized, select electrochemical deposition of  $\text{Sc}(0)$  can be developed from the IL. Little information is available to direct these fundamental electrochemical studies but literature reports support this as a reasonable approach.

The results of this effort include:

- Identified an efficient and more cost-effective method for dissolving scandium *and* erbium metal
- Developed paths for changing scandium structure to allow us to tune solubility and electrochemistry in ILs
- Identified a method for Sc and Er reduction that allows for recovery of pure Sc/Er in a cost effective and environmentally benign way

These results can contribute toward ensuring a reliable supply of critical elements for DOE and DoD applications and could help alleviate potential future supply disruptions.



## Trust Verification Platform (Trust of Third Party Digital Design Tools using Formal Methods)

180931 | Year 2 of 3 | Principal Investigator: T. Mannos

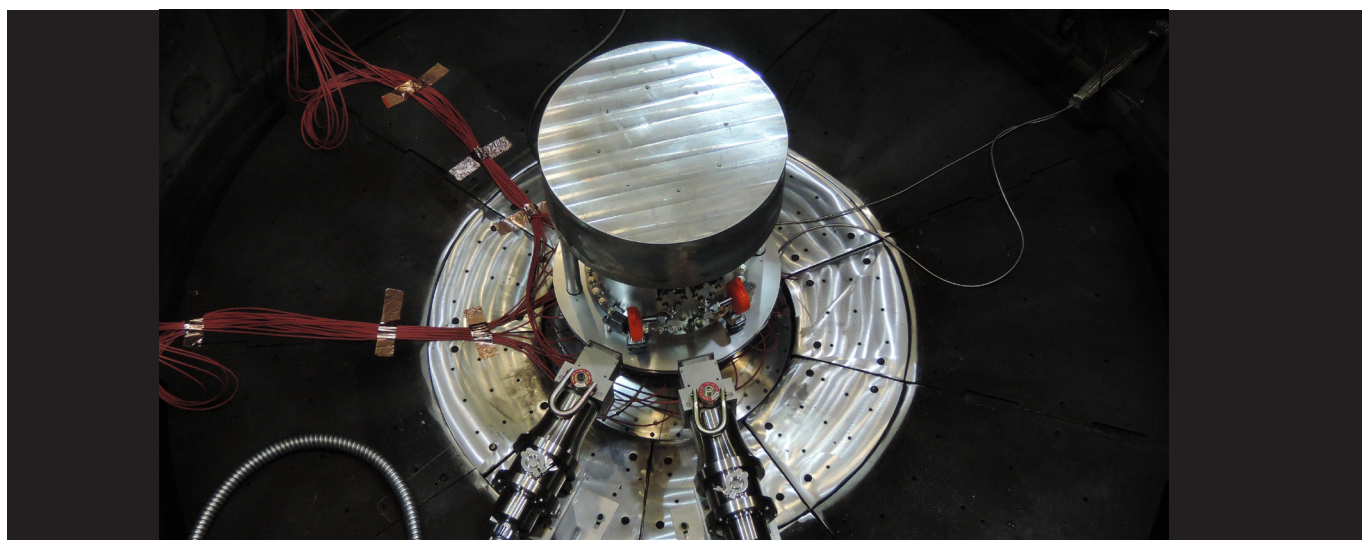
### Project Purpose:

This project is developing a trust verification platform (TVP) to verify the integrity of application-specific integrated circuit (ASIC) design and implementation output files for trust. Digital ASICs start with an abstract description of the design either in register-transfer level (RTL) or a high-level synthesis (HLS) language. This is then synthesized to logic gates, placed and routed, and prepared into a GDSII format for handoff to the mask provider. The mask provider further transforms the GDS by fracture and optionally addition of optical proximity correction (OPC) features such as serifs, then hands the result back to the design agency in a mask data format (e.g., MEBES).

Historically, it has not been common practice for design organizations to perform formal or exhaustive checking of the mask data prior to fabrication. TVP closes the loop by extracting a gate-level netlist from the GDS file and comparing the result to the source (RTL) using formal equivalence. It also performs a static timing analysis to determine if any timing violations were introduced during implementation or translation. We have successfully tested the process on production designs of up to 8600 registers and developed enhancements to enable scaling to arbitrarily-sized ASICs. In the final year of the project, we will explore verification options beyond GDS and begin final evaluation including red teaming to expose any weaknesses in the technique. Metrics will be collected and optimized include false positive rate, measure of agreement among numerical outputs (e.g., Lin's concordance correlation coefficient), and red team success rate



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## Grand Challenges

Grand Challenges are bold, game-changing ideas with the potential for enormous impact to the security of the nation through significant advances in science and engineering. Grand Challenge projects are expected to drive the future of Sandia by providing new directions, capabilities, and solutions and to provide long-term impact to multiple programs. These projects result in a long-term ST&E legacy for Sandia from breakthrough scientific discoveries through development of unique and differentiating technical capabilities. These projects are multimillion dollars in size and utilize multidisciplinary teams, often including external collaborators.

*In the image above, two fast neutron radiation-effects cassettes aim toward the center of the containment system for tritium within Sandia's Z vacuum chamber. The setup's gas transfer system is housed within the containment system. (Project 173104, New Capabilities for Hostile Environments)*

## Projects

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## Changing the Engineering Design and Qualification Paradigm in Component Design and Manufacturing (Born Qualified)

191144 | Year 1 of 3 | Principal Investigator: R. A. Roach

### Project Purpose:

The nuclear weapon (NW) enterprise requires transformative approaches to the stockpile that promote assurance, affordability, and agility to retain a safe, secure, and effective nuclear deterrent. Today, it takes roughly 12-15 years to introduce new technologies into the NW stockpile. In addition, the lack of tightly controlled and automated manufacturing tools and processes has led to largely artisan-based design and manufacturing processes that when combined with the requirement for high reliability and long development lead times, results in cost inefficiencies, loss of flexibility and agility, and adequate but incomplete quantification of performance margins and reliability.

Our goal is to revolutionize the component engineering design, manufacturing, and qualification paradigms. The vision for product realization is a paradigm shift realized via additive manufacturing (AM) processes where margins to requirements, limits of physics, and process uncertainties are known at birth, and product changes can be swiftly propagated through the design-manufacture-sustainment chain to assess impacts. With the simultaneous creation of part and material, AM breaks down the traditional walls between the disciplines of materials assurance and part certification providing a unique opportunity to drive changes in the qualification paradigm. Our approach is hierarchical and science-based, where we first acquire foundational knowledge of materials, then progress to next-level assemblies to achieve component qualification. AM techniques will expedite material design for component performance. Modeling and simulation with optimization and uncertainty quantification will allow margin quantification, uncertainty minimization, and identification of critical performance parameters.

This project addresses the following technical challenges:

- Novel real-time AM diagnostic tools to quantify and monitor critical AM process variables for control and optimization
- Innovative experimental techniques to provide real-time materials assessment
- Models to relate microstructure to bulk properties to enable translating AM process results to material properties
- Approaches to incorporate material and process variability into AM process models
- Intelligent data collection from various diverse sources to develop deep physical understanding





## Fundamental Trust Analysis

191147 | Year 1 of 1 | Principal Investigator: B. K. Eames

### Project Purpose:

The US government has repeatedly demonstrated the effectiveness of technology as a means of establishing safety and security and achieving new mission capabilities. However, the increasing dependence on commercial technologies exposes government systems to potential malicious alterations during the development process. Can these systems be *trusted* to perform their intended function when called upon?

The trust issue is pervasive and has proven elusive to structured science/engineering approaches that aspire to deflect malicious alterations. In the absence of a system of science supporting trust, the government employs opinion-based risk assessments, red team analysis, and system access denial to increase confidence that systems will perform as intended. Confidence is based upon certification, waiver and opinion-based analysis rather than quantifiable, engineering-based approaches to evaluate and endow trust.

We propose to define foundational techniques for supporting analysis of trustworthiness and for improving trust through diversification. Specifically, we propose to build on existing research in game theory, supply chain analytics, and risk assessment to develop a novel graph-based game-theoretic approach for analyzing trust. We will develop verification-based analysis techniques to identify effective ways to apply diversity. This research, if successful, will advance the ability to conduct quantitative analysis of trust, and will lay the groundwork for future development of objective techniques for the analysis and synthesis of trust.

Measuring and engineering trust presents difficult research problems with national-scale impact. Sandia is ideally suited to address these complexities due to its long history of developing highly reliable systems and understanding nation-state threats.

## Hardware Acceleration of Adaptive Neural Algorithms for Dynamic and Intelligent Threat Detection

180885 | Year 2 of 3 | Principal Investigator: C. D. James

### Project Purpose:

In the face of exponentially increasing data and saturated microprocessor speeds, new technology approaches are needed to identify and analyze modern sophisticated threats. Historically, algorithm theory and hardware implementation have been separated tasks, often leading to inflexible algorithms mapped to overly specialized hardware. The Hardware Acceleration of Adaptive Neural Algorithms (HAANA) Grand Challenge project is generating novel neural-inspired algorithmic approaches toward detecting threat activity in the cybersecurity and remote imaging domains, with a specific interest in intelligent threats that adapt over time and engage in evasive behavior. This project is designing neural-inspired machine learning algorithms, and formulating hardware at the device and system architecture level to provide real-time, adaptive, threat recognition. The algorithms core has a three-pronged strategy for the use of neural-inspired algorithms in cyber and remote imaging domains: 1) utilize temporal coding to improve data sampling and reduce power/cost, 2) leverage adaptive algorithms to handle time-evolving variations in multiple streams of data, and 3) demonstrate the strength of sparse coding for processing large volumes of data and extracting useful threat signatures. The architecture core has implemented a neural-inspired architecture in conventional technology to demonstrate improved speed for combing through large volumes of cyber data and identifying specific data patterns of activity of interest. The learning hardware devices core is currently simulating a resistive memory architecture for incorporating offline and online learning with highly dense and low-power analog computation processing. The device design and fabrication is being directly guided by modeling to optimize the speed of algorithm training and the accuracy of algorithm performance.

Given the explosion of data in the cyber and remote imaging domains and the saturation in microprocessor speeds, the codesign of algorithms, architectures, and device hardware is needed to handle modern sophisticated threats. This basic research in algorithms and device hardware required for accelerating the adaptive learning of threat signatures in complex multimodal data is ideally suited for LDRD investment.



## NanoCRISPR: A Revolutionary Therapeutic Platform for Rapidly Countering Emerging and Genetically Enhanced Biological Threats

190245 | Year 1 of 3 | Principal Investigator: D. Y. Sasaki

### Project Purpose:

Two urgent problems currently threaten national and global biosecurity: 1) the accelerating emergence of highly virulent, transmissible, drug-resistant pathogens, and 2) globally available, low-cost tools for creating and reengineering organisms, which greatly increase the odds of accidental or intentional manufacture and release of deadly pathogens. The hallmark of these biothreats is genetic novelty that evolves naturally or is introduced deliberately to enhance virulence and multi-drug resistance, rendering existing countermeasures ineffective. To address the looming threat of these organisms, the US Department of Health and Human Services Secretary has stated that, 'Our nation must have the nimble, flexible capacity to produce medical countermeasures rapidly in the face of any attack or threat, known or unknown, including a novel, previously unrecognized, naturally occurring emerging infectious disease.' To solve this problem, we propose to develop what we term 'NanoCRISPR,' a rapid, cost effective, universal technology for identifying and delivering potent new medical countermeasures against emerging and engineered biological threats. We will utilize CRISPR, a recent, revolutionary discovery that was voted Science magazine's '2015 Breakthrough of the Year' due to its ability to edit target genes in a highly controlled manner, to develop novel pathogen and host-directed countermeasures. We will then package CRISPR components within state-of-the-art nanoparticle delivery vehicles developed at Sandia and modulate various nanoparticle properties, including size and surface modifications, to deliver them to specific organs, promote their uptake by pathogen-infected cells, and release them within appropriate intracellular locations in order to achieve targeted cleavage of pathogen RNA/DNA or targeted disruption of pathogen-host interactions.

## New Capabilities for Hostile Environments

173104 | Year 3 of 3 | Principal Investigator: P. J. Griffin

### Project Purpose:

The purpose of this project was to develop new physical simulation capabilities in order to support the qualification of nonnuclear weapon components in hostile radiation environments. The project contributes directly to the goals of maintaining a safe, secure, and effective US nuclear stockpile, maintaining strategic deterrence at lower nuclear force levels, extending the life of the nuclear deterrent capability, and to be ready for technological surprise.

Our approach was to develop fast neutron and warm x-ray sources and provide radiation effects testing environments on the Z Pulsed Power Facility that will fill gaps in presently available experimental capabilities at fluences and spectra of interest and over object sizes of interest to stockpile qualification. These new capabilities will enable the stockpile modernization program to take advantage of risk-informed trade-offs between margin, cost, schedule, and hardness for the design and qualification of advanced technologies.

The technical path leveraged the advances made in our understanding of the physics and performance of classified z-pinch targets over the last six years. Development of the sources requires the use of innovative ways to increase the delivery of current to z-pinches, further advances in the target design of warm x-ray and neutron sources, and development of an innovative scientific and engineering basis to safely use tritium on the Z Facility. Equally important, the development of warm x-ray and fast neutron science platforms on Z allows the fielding and diagnosis of powered and actively probed circuits during Z.

This project utilized a dual-pronged approach to develop experimental platforms and innovative neutron and x-ray sources that bridge present and forecasted gaps in nuclear weapons mission space. This work significantly enhances our capability through iterative development cycles of theory, simulation and design coupled with experiments on Z to validate innovative source designs, and development and fabrication coupled with experiments on Z to validate experimental configurations and advanced diagnostics.



## Revolutionary SWaP Capability from Ultra-Wide-Bandgap Power Electronics

180884 | Year 2 of 3 | Principal Investigator: R. Kaplar

### Project Purpose:

The purpose of this project is to create and demonstrate novel approaches to improve the size, weight, and power (SWaP) characteristics of power conversion systems and to demonstrate their robustness in harsh environments. This is a critical need broadly crosscutting both the civilian and defense sectors. To this end, the project is developing the next generation of materials and power switching devices based on ultrawide-bandgap (UWBG) aluminum gallium nitride (AlGaN) semiconductors, leapfrogging current power electronics technology. In so doing, it will enable orders-of-magnitude SWaP advances in power conversion systems for multiple national security mission areas. The project consists of four complimentary and integrated thrusts: 1) UWBG materials development, focused primarily on epitaxial growth, 2) novel design and fabrication methods for high-power UWBG devices, 3) understanding and eliminating defects (including radiation-induced defects) that degrade performance and reliability, and 4) characterizing device performance in power conversion environments, and prototyping novel demonstrations for exemplar application needs. The four thrusts are integrated through the common vision of developing two specific categories of power devices, vertical and lateral, both of which will exceed today's state of the art in terms of quantitative metrics such as breakdown voltage, on-resistance, and switching time. The development of each type of device requires coordinated expertise from each of the four thrust areas. Our approach is science-based, whereby fundamental physical understanding rooted in experiments, theory, and simulation is leveraged to provide a long-term foundation for reliable, high-performance power semiconductor devices. Sandia's enduring world-class expertise in wide- and ultrawide-bandgap materials uniquely positions us to overcome the challenges in developing this next generation of power semiconductors. Collaborations with government, industry, and university partners are extending our capabilities.

## Sandia Enabled Communications and Authentication Network using Quantum Key Distribution (SECANT QKD)

173103 | Year 3 of 3 | Principal Investigator: R. Camacho

### Project Purpose:

Quantum information science has the potential to dramatically change the national and international landscape in communications, sensing, and computing. Among these, quantum communications technologies are the most advanced with the greatest potential for near-term impact. In particular, quantum key distribution (QKD) has received significant investment from international government and industry sponsors with the hope of enabling theoretic unconditional information security. Current communications security relies on widely accepted (though never proven) beliefs in the difficulty of solving certain mathematical problems, while QKD uses the laws of quantum mechanics to establish secret cryptographic keys.

All previous QKD systems relied on bulky table-top devices, which presented two major drawbacks for wide-scale adoption. First, owing to their large size, weight, power and cost, these systems were neither scalable nor compatible with current communications network infrastructure. Second, and perhaps more importantly, in spite of theoretic proofs of unconditional security, imperfections in bulk-optics QKD hardware were shown to be vulnerable to sophisticated cyber attacks.

The SECANT project developed and demonstrated the first microfabricated quantum transmitter/receiver. The system miniaturizes all of the components necessary to securely encode, transmit, receive, and decode quantum photonic signals onto a single microchip, in effect creating an ultra-secure cryptographic network node for secure communication or network applications. This new technology accomplishes what bench-scale quantum encryption systems do but at one millionth the scale, on a chip roughly 3 mm x 5 mm and weighing less than an ounce.

To enable the chip's operation, several discoveries and world-firsts were also demonstrated, including waveguide-based single photon detectors, on-chip optical polarization processing, low-loss fiber-to-chip coupling, numeric QKD security proofs, and efficient new QKD protocols.

Along the way, the SECANT team also discovered that the innovations required to put QKD on a chip can also enable many other previously unavailable technologies for applications including quantum physical security, energy grid security, deep space quantum communication, quantum-limited imaging, and distributed quantum computing.



## Smart Sensor Technologies

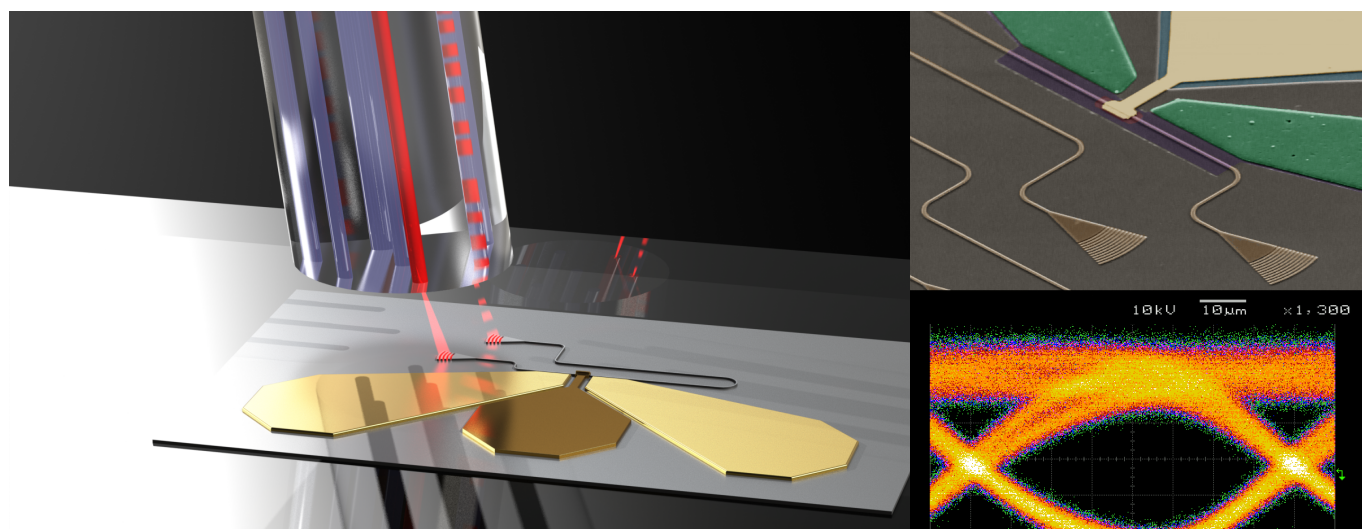
189614 | Year 1 of 3 | Principal Investigator: D. W. Peters

### Project Purpose:

Sensing is vital for many tactical and strategic applications—alerting warfighters or decision makers to the occurrence of an event. There is a continuously increasing demand for greater and more relevant information from these sensor platforms. For infrared sensing, the physical sensor has become the limiting factor in improving data delivery to the end user, as current infrared detector architectures approach their fundamental noise floor.

For satellite systems, the problem is worsened by the expense, long development times, and long lifetimes of missions. It is impossible to predict the necessary capabilities to monitor threats that will appear in even a few years' time. Fixed, single mission remote sensing space systems risk being outdated by new threats even before deployment. There is an urgent need for highly sensitive systems that reconfigure themselves on-the-fly, intelligently respond to scene changes as events happen, and adapt to mission needs as threats evolve, while providing high quality data.

The Smart Sensor Technologies (SST) Grand Challenge project seeks to fill this need—offering fast, agile spectral bandwidth control *at the pixel level*, while simultaneously offering increased sensitivity well beyond the current limit. Such a real-time, pixel-level, spectrally tunable sensor will provide high information content multispectral imagery that meets the needs of many different mission areas and will be capable of adapting to new threats or entirely new missions. Our revolutionary approach breaks the current focal plane array paradigm, has the potential to revolutionize the industry, and could greatly expand Sandia's contributions to the remote sensing community.



## Exploratory Express

The Exploratory Express Investment Area provides a mechanism for maturation and testing of a novel idea that has potential to become very important for one of Sandia's strategic missions. This Investment Area was initiated to provide a vehicle to explore novel ideas that are generated by researchers spontaneously through the year rather than in response to a specific proposal call. Proposals may be submitted throughout the year with the selection of funded projects occurring three times each year. A small amount of funding ( $\leq \$100K$ ) is provided to Exploratory Express projects over a period of no more than a few months to address one critical question as the basis for determining whether the idea is desirable for Sandia to pursue more thoroughly to mature its strategic importance for Sandia's national security missions.

*The photos above show the first demonstration of a high-speed nanophotonic modulator based on carrier density modulation in transparent conducting oxides. (left) Integrated modulator. (top right) Colorized scanning electron microscope image of the fabricated device. (bottom right) 2.5 billions of bits per second eye diagram. This research focused on establishing a clear path to the creation of efficient, ultrafast nanoplasmonic modulators, which would be of use to many national security applications (Project 192700, Probing Charge Layers in Conducting Oxides for Next-Generation Plasmonics)*

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## A Nanocomposite Inductor for Pulsed Power Fusion

191316 | Year 1 of 1 | Principal Investigator: D. L. Huber

### Project Purpose:

Linear Transformer Drivers (LTDs) are an important new technology that is critical for the future of pulsed power, including applications such as energy production from fusion. However, LTDs are currently very expensive and there are significant risks in scale-up of production. Much of this risk is in the production of the inductor cores needed for LTDs. An alternate technology would be the production of an iron nanocomposite that can yield higher saturation magnetization, higher susceptibility, and no hysteresis. This new nanocomposite material would lower parasitic current losses and remove a magnetic reset step that is required with current cores leading to electrical efficiency improvements of 5-10%. While the basic chemistry and physics of this material has been worked out, a 1/10 engineering scale toroid must be produced to allow realistic tests of the material in a relevant environment. This is a significant undertaking, but without this step, the technology will remain stuck at a very low technical readiness level.

This project seeks to quickly scale up production of nanocomposite by approximately two orders of magnitude, followed by fabrication of three toroid inductors for testing using existing capabilities. It is not clear how the components will behave in a nanocomposite material. Scale-up of production is also a significant risk. The technical approach is designed to address these risks.

## Artificial Diffusion: Rapid Disease Detection by Driven Magnetic Polybeads

195557 | Year 1 of 2 | Principal Investigator: J. E. Martin

### Project Purpose:

Immunoassays are an effective method of determining if an individual has been exposed to an infectious disease. However, these assays are typically very slow due to the long incubation time for the formation of antigen-antibody complexes in viscous media, such as blood plasma. Because the assays are typically done in microtiter plates, mixing is ineffective due to the low Reynolds number in the small wells, which can be as small as 10 nanoliters. The goal of this project is to use magnetic fields to create *artificial diffusion* that will greatly accelerate the rate of antigen-antibody complex formation. Our project takes advantage of the fact that a standard approach to immunoassays uses antibody-coated magnetic polybeads to complex with specific antigens that indicate disease exposure. These antigens are functionalized with a fluorescent dye. After exposure to the solution containing the antigen-dye conjugate, the polybeads can be extracted with a magnet and the residual luminescence determined. The intent of this project is to accelerate the binding kinetics by using *triaxial magnetic force fields* to drive the paramagnetic polybeads on structured "ergodic" journeys through the solution, seeking out and binding the antigens that are specific to the antibody bound to the polybeads. We can optimize both the search volume and the bead velocity by controlling the strength and frequency of each of the field components.



## Artificial Graphene in Undoped Semiconductor Heterostructures

192794 | Year 1 of 1 | Principal Investigator: T. Lu

### Project Purpose:

Graphene is a unique 2D electron system in that the electrons are massless due to the linear energy momentum dispersion. This linear dispersion arises from the honeycomb lattice potential. Lateral superlattice with triangular symmetry superimposed on a conventional 2D electron system, in principle, produces the same linear dispersion and makes the so-called artificial graphene. To date, there have only been a few experimental studies presenting evidence of artificial graphene using optical probes. No electrical transport measurement has been reported, presumably due to material limitation of modulation-doped heterostructures.

At Sandia, we have a long history of producing 2D electrons and holes in undoped semiconductor heterostructures (GaAs/AlGaAs and Si/SiGe) and we engineer them for electron physics research. Prior results from a Si/SiGe undoped heterostructure with a square superlattice gate show superlattice induced effects in transport. We plan to produce a 2D electron system in undoped semiconductor heterostructures (GaAs/AlGaAs and Si/SiGe) with electronic properties of graphene and detect them electrically. We, thus, plan to fabricate undoped field-effect transistors with honeycomb superlattice gate and detect the linear dispersion through transport measurements. The linear dispersion will manifest itself in the zero-field resistivity and the Hall resistivity, as well as the degeneracy and gaps in the quantum Hall regime. The characteristics will allow us to definitely demonstrate artificial graphene.

Engineering artificial graphene using undoped semiconductor heterostructures has never been demonstrated before. Due to the sensitivity of the band structure to disorder, it requires high, quality starting material, demanding high, resolution nanolithography, reliable semiconductor processing, and a substantial understanding of enhancement-mode devices. Characterization of the fabricated devices also requires nontrivial cryogenic measurements.

## Auto-Magnetizing (AutoMag) Liners for MagLIF: Helically-Wound Composite Liners

195306 | Year 1 of 1 | Principal Investigator: T. J. Awe

### Project Purpose:

In Magnetized Liner Inertial Fusion (MagLIF), premagnetized and preheated fusion fuel is compressed to fusion conditions by a magnetically imploded liner (tube). Premagnetization reduces conduction losses from the hot fuel; this is currently accomplished using an external Helmholtz-like coil pair. The coils must rise slowly (3 milliseconds) so that the field diffuses through the liner without crushing it. During the slow rise, the coils must withstand forces of order 500,000 pounds and mechanical failure limits the maximum deliverable field to 30 Tesla (T). Furthermore, to deliver fields in excess of 10 T, the growing wound-copper-coil cross section significantly restricts diagnostic access to the MagLIF liner. Finally, the coils require a high inductance current feed which limits the peak current to the MagLIF liner to ~18 Mega amps, MA. In comparison, Z has delivered ~25 MA to lower inductance loads. In this project, we intend to explore the novel "AutoMag" concept which uses a helically wound metal/dielectric composite liner to premagnetize the fuel in MagLIF, and eliminates the external field coils and all concerns discussed above. The AutoMag liner premagnetizes the fusion fuel in ~100 nanoseconds; therefore, mechanical failure is of little concern, and fields significantly exceeding 30 T can be likely be achieved (limited by dielectric breakdown). Next, AutoMag liners are composed of low opacity materials (beryllium and plastic) so hard x-ray diagnostic access is unimpeded. Finally, AutoMag can be driven by a low inductance feed, enabling significantly increased load current delivery. AutoMag has great potential to be transformational for MagLIF on both Z and on next-generation pulsed power facilities.



## Fracture Toughness of Microstructural Gradients

193072 | Year 1 of 1 | Principal Investigator: C. C. Battaile

### Project Purpose:

Conventional fracture mechanics assumes homogeneous, isotropic materials, which leads to toughness estimates that are inaccurate in parts with microstructural and/or thermodynamic gradients. Therefore, existing structural assessments are based on approximate material properties that produce incorrect predictions of the true fracture driving force. Whether through the unavoidable effects of materials processing, or through intentional design, most engineering components are graded or anisotropic in some way, for example by solidification, texture, or chemistry. Ongoing activities in damage and failure analysis at the engineering scale cannot afford the sort of fundamental effort required to address this problem, and much of Sandia's research efforts in the area of fracture and failure are devoted to assessing the validity and predictability of the many conventional approaches that exist in this regard, but that only apply to homogeneous materials. We will pursue an exploratory effort to ascertain the potential and possibility of extending existing fracture mechanics models to account for gradients and anisotropy. The concept of a generalized, inhomogeneity-aware fracture model is largely uncharted territory. It is unclear how or if this shortcoming in existing fracture theories can be remedied tractably.

## High Brightness, Room Temperature III-Nitride Based Single Photon Source

195215 | Year 1 of 1 | Principal Investigator: G. S. Subramania

### Project Purpose:

Single photon sources (SPS) are quantum light sources where photons are emitted one at a time instead of randomly (e.g., lasers) or in a bunch (e.g., thermal). Highly desirable features of SPS include the abilities to exhibit deterministic emission, electrically injected room temperature operation with high photon rate, high extraction efficiency, and controllable directionality. Approaches taken thus far using different material systems have only addressed a subset of these features. A III-nitride based approach offers a clear pathway to deterministic, room temperature, electrically injected practical SPS, as one can potentially also leverage the knowledge and technology from the light emitting diode world. In this project, we will explore, understand, and potentially overcome a key challenge—achieving low gain ( $g_2 < 0.2$ ), room temperature SPS with high extraction ( $\sim 40\%$ ) based on a III-nitride quantum dot deterministically placed inside a photonic crystal cavity. We will use a hybrid approach wherein a  $\text{TiO}_2$ -based photonic crystal cavity will be fabricated around an InGaN quantum dot (QD) embedded nanoscale post utilizing Sandia's prior expertise in these areas. Optimization of the cavity design to achieve high quality factor, mode overlap with QD, and high extraction will be guided by finite difference time domain simulations. The single photon behavior of the structures will be characterized using a Hanbury-Brown Twiss spectroscopy system. Success is expected to lead to high impact publications and can be game changing for quantum computing, secure communications, and quantum-level detection metrology.

## Hyper-Insulating Fullerene Inks For Thermal Barrier Coatings

198383 | Year 1 of 1 | Principal Investigator: B. J. Kaehr

### Project Purpose:

Extremes of heat conduction have been realized by manipulating the heat carriers on the atomic scale. For example, while 2D materials such as graphene have proven to be exceptional thermal conductors, weakly bonded systems have demonstrated the ability to be "hyper-insulating," achieving thermal conductivities below the amorphous limit. Recent work has shown that phenyl-C61-butyric acid methyl ester (PCBM), a fullerene derivative, exhibits exceptionally low thermal conductivity. This class of materials has not previously been considered for thermal applications. Indeed, 20 years after the Nobel Prize was awarded for discovery of this carbon allotrope, the true promise of fullerene materials may, in fact, be their development as ultra-thin, high-efficiency thermal barrier coatings that can be printed in a range of form factors to develop (flexible) electronics, pyroelectrics, thermoelectrics, and next-generation thermal barriers. Given the higher thermal conductivity of  $\text{C}_{60}$  films versus PCBM (a factor of 3 lower), we started with the hypothesis that longer side chain functional groups effectively decreases the vibrational frequency to yield lower thermal conductivity solids compared to  $\text{C}_{60}/\text{C}_{70}$ . In this work, we experimentally observed the opposite effect, specifically, increasing the side chain mass/size increased thermal conductivity. This is partly explained via boundary conductance measurements and molecular dynamics (MD) simulations of fullerene derivatives in solution. Overall, this work defines a path forward to develop tunable and printable fullerene based inks for thermal barrier applications.



## Improving Catalysis with Bifunctional Conductors

195216 | Year 1 of 1 | Principal Investigator: T. N. Lambert

### Project Purpose:

Efficient catalysis of the oxygen reduction reaction (ORR) is critical to the development of renewable energy technologies such as fuel cells and metal air batteries. High over-potentials are associated with the complex four-electron transfer of the ORR, increasing operating potentials. Current commercial electrocatalysts for the ORR are also based on rare precious metals such as Platinum/Carbon (Pt/C), which are expensive and not environmentally sustainable. Thus, there is motivation to design materials with the ability to catalyze the ORR that do not incur such high costs nor sacrifice resources. This project examined new approaches to developing next-generation oxygen ORR catalysts based on organic-inorganic hybrid electrocatalysts. We recently disclosed that hybrid thin films based on co-electrodepositing manganese oxide and the intrinsically conductive polymer (ICP) poly(3,4-ethylenedioxythiophene, PEDOT) are competitive with the commercial benchmark catalyst 20% Pt/C as electrocatalysts for ORR in alkaline electrolyte. Based on this success, we set out to better understand the synergistic effects and examine new, more flexible synthetic approaches to this class of materials and prepare new intrinsically conductive polymers (ICPs) that would allow for fine tuning the electronic and ionic properties of the polymer.

## Ionic Borate-Based Covalent Organic Frameworks: Lightweight, Porous Materials for Lithium-Stable Solid-State Electrolytes

195217 | Year 1 of 1 | Principal Investigator: H. T. Black

### Project Purpose:

Lithium metal provides an exceptionally high energy density alternative to traditional graphite anodes and is currently under intense investigation for use in lithium ion batteries. However, the high reactivity of lithium leads to undesirable side reactions and dendrite growth that degrade device performance and can lead to catastrophic failure. Therefore, there is an urgent need for lithium-stable solid state electrolytes (SSEs) and/or ion conductive protection membranes in order to improve the lifetime and safety of lithium anode batteries. The controlled pore size and tunable pore chemistry of covalent organic frameworks (COFs) make these materials exceptional candidates for use as SSEs in lithium anode batteries, where ion conductivity can occur via transport within the pores. On the other hand, COFs generally exhibit poor stability due to the relatively weak chemical bonds that are formed during their synthesis. This has prevented COF materials from being used in lithium anode batteries. Furthermore, only a small set of reactions are known for the synthesis of COFs and ionic COFs have never been reported. This project presents a strategy for synthesizing the first ionic COFs with thermodynamic stability toward lithium metal. The approach relies on transformation of a well-known boroxine COF into its anionic borate form, which is known to exhibit exceptional stability in small-molecule analogs. Meanwhile, the chemical transformation will result in an ionic COF structure that is expected to afford good ion conductivity. Successful preparation of this COF will uncover a novel platform of SSE materials for use in lithium anode batteries.





## Measuring Idea Generation and Test

193073 | Year 1 of 1 | Principal Investigator: J. Y. Tsao

### Project Purpose:

We have hypothesized that the fundamental engine of the evolution of complex adaptive systems is generation and selection. In biology, it is the reproductive generation of organisms with some variation, followed by selection of those organisms that are best adapted to their environment. In business economics, it is the generation of companies which sell various products, followed by selection of those whose products are most profitable. In knowledge production, it might be something akin to idea generation and selection, possibly analogous to information entropy (or uncertainty) creation/destruction.

In practice, however, the connection between the abstract notion of idea generation/selection and how we as human beings operationalize idea generation/selection has been difficult to bridge. Idea generation/selection contains many moving parts, and until it is broken down mechanistically into those moving parts, it seems difficult to devise experiments and measurements for testing this overall hypothesis.

In this project, we developed a simple and, we believe, intuitive model for idea generation and selection. The model's simplicity enables it to be mechanistic and to be expressed mathematically, and thus enables one to see at least semi-quantitatively how its pieces interact with one another in service of the overall whole. We are cautiously optimistic that the mechanisms in the model might be connected eventually to individual, group, and institutional behaviors, thus possibly enabling testing (falsification) of the model as well as quantitative diagnosis and improvement of those behaviors.

## Modeling Electric Double Layer Effects on Charge Transfer at Flow Battery Electrode/Electrolyte Interfaces

192869 | Year 1 of 1 | Principal Investigator: K. Leung

### Project Purpose:

The project aims to model interfacial processes associated with redox flow batteries (RFB) for grid/stationary storage, with the ultimate goal of helping design new electrolytes, electrodes, redox species, and interfaces. It addresses the linked problems of electric double layer (EDL) structure and electron transfer at model electrode/electrolyte interfaces. Fast electron transfer partly determines which redox species are viable for flow batteries, along with solubility, viscosity, and other factors. Commercial systems apply aqueous, vanadium-based complexes, but other choices and organic electrolytes with larger voltage windows are the subject of active research at Sandia and elsewhere. The high salt concentration present in flow battery electrolytes yields nontrivial EDL consisting of solvents, counter-ions, co-ions, and redox species, existing with different charge states at the charging voltage threshold. EDL strongly influences electron transfer, especially when redox "mediators" are used. Modeling this key missing information is the main challenge. Our project seeks to apply Sandia's LAMMPS molecular dynamics code. As a proof of principle, we will study minimal model systems consisting of a graphite electrode with ferrocene and fluoronone as redox-active species. These model "catholyte" and "anolyte" molecules exhibit low reorganization energies (in the sense of Marcus theory) and are most amenable to EDL simulations which involve switching of redox states to mimic electron transfer. This study will enable future modeling and design of redox species relevant to flow batteries and redox mediators.



## Normalized Compression Distance as a Metric for Analytic Software Utility

198367 | Year 1 of 1 | Principal Investigator: L. A. McNamara

### Project Purpose:

This research examined information theoretic measures as a robust, broadly applicable, repeatable metric for comparative assessment of data analysis systems aimed at helping users reduce high-dimensional data into topically relevant subsets of information. The information theoretic measure we have selected for testing was a normalized information compression distance (NCD), which is a feature- and parameter-free way of evaluating the similarity of two or more information objects. The simplicity and generalizability of such compression-based measures lend them to a wide range of applications as a process measure of information interaction in visual analytic systems.

Evaluation guidance in the InfoVis/VA (visual analytics) community has emphasized “insight” as an outcome measure for assessing the benefit of VA systems for human workflows. Insight-focused evaluations have tended to rely on whether participants solve test problems and/or whether they report an insight event. The drawback to such “insight” oriented evaluation studies is that “insight” is a highly subjective outcome that is difficult to measure; it also involves multiple perceptual and cognitive subprocesses that are not well understood nor easily measured.

We suggest a different approach to the problem of evaluating VA systems: rather than focus on outcomes, such as problem solution or “insight” events, we suggest that all human workflows involving large datasets necessarily require people to reduce the amount of data they are working with to a tractable, comprehensible level of information. This information reduction process is directly measurable in information theoretic terms, which, thanks to Claude Shannon’s formulation, provide a context and content independent way to assess changes in the complexity of an information set.

## Optimization of SiV Defect Yield in Diamond Substrates

192701 | Year 1 of 1 | Principal Investigator: E. S. Bielejec

### Project Purpose:

Color centers (defect complexes such as silicon vacancy center [SiV]) in diamond have shown potential in fields such as metrology, cybersecurity and quantum computation. Demonstrations in these fields have pushed the envelope of state-of-the-art operations—for example, single photon sources (SPS) making use of SiV centers in diamond for quantum key distribution have demonstrated all the requirements for SPS operation including: 1) stable operation with second correlation function  $\ll 1$ , 2) electrically driven single photon emission, and 3) compatibility with frequency conversion to telecommunication frequencies. To date, however, all these demonstrations have been on lab-scale one-off devices. The key question behind how to deterministically fabricate these devices, namely activation yield, has been overlooked. For context, Si-based semiconductor devices are vastly successful because we have a high activation yield for implanted dopants. This is not yet true for diamond color centers. As currently understood, the color center yield is dominated by a lack of vacancies in the immediate area of the implantation. We seek to optimize the activation yield of color center using a combination of: 1) focused single ion implantation with in situ detection to count the number of implanted Si ions and 2) localized point defect (vacancy) creation using a focused Li ion beam to improve the yield. These experiments build on the unique capabilities of the Sandia nanoImplanter (nI) to produce focused ion beam with spatial resolution of  $< 10$  nm of both silicon and lithium ions. This work will also leverage our world-leading single ion implantation and detection capabilities. The project is relevant to DOE’s Scientific Discovery and Innovation mission, with potential benefit to others.



## Porous Liquid Electrolytes for Metal-Air Batteries

198370 | Year 1 of 1 | Principal Investigator: F. S. Gittleson

### Project Purpose:

Metal-air or metal-oxygen batteries represent the next generation of power on demand technologies with energy densities 2-3 times greater than Li-ion. Despite potential uses in electric vehicles and portable electronic devices, the practical application of these systems is hampered by physical properties related to the nonaqueous electrolyte. To date, electrolyte "design" has largely been a trial and error process of evaluating known species, but understanding the criteria for high power and energy density may allow us to generate novel task specific electrolytes.

In metal-air batteries, there exists a critical 1:1 relationship between oxygen solubility in liquid electrolytes and power/energy density, which, if exploited, can improve device performance by an order of magnitude. By systematically varying the molecular structure of electrolyte solvents, solubility and its coupled property of diffusivity, can be optimized to enhance oxygen transport. Controlling both the size and polarity of electrolyte molecules are two potentially profitable methods to enhance these properties. Ionic liquids, a class of organic molten salts that are defined by their low melting point, offer a platform to evaluate the effect of tuning molecular structure.

To date, there has been little effort to understand and engineer better mass transport in metal-air battery electrolytes. The goal of this project is to obtain valuable insight into fundamental phenomena that should enable new energy storage technologies.

## Probing Charge Layers in Conducting Oxides for Next-Generation Plasmonics

192700 | Year 1 of 1 | Principal Investigator: G. A. Keeler

### Project Purpose:

Plasmonic approaches to optical signaling promise order-of-magnitude size reductions beyond conventional photonic limits, and could enable revolutionary improvements in power dissipation, integration density, and functionality for computing, sensing, and communications. Recent reports of compelling plasmonic modulators suggest that they may be the first practical, high-speed nanoplasmonic devices. These modulators operate by strongly altering the carrier density of conducting oxide layers. Such films are not traditionally used in high-speed photonics, and materials limitations (including leakage current filaments through dielectric layers or charge trapping at grain boundaries and interfaces) may explain why experimental work to date has failed to demonstrate even moderately high-speed switching. The goal of this project was to study the dynamics of the essential charge layer in high-quality conducting oxide films to assess the feasibility of efficient, ultrafast plasmonic modulators.

This project explored the key physics and practical limitations of controlling charge carrier density in thin conducting oxide layers, with the goal of enabling next-generation plasmonic devices with high potential impact. Specifically, this work looked to demonstrate that sufficiently large carrier densities can be obtained in the conducting oxide films, that dielectric leakage paths are nondominant sources of carrier density, and that electron accumulation layers can be created and removed at high speeds. These topics further our scientific understanding of materials and interface limitations for oxide-based plasmonic devices, and highlight a path to compelling practical devices with significant potential impact on DOE-relevant mission areas, including compact, ultrafast, low-power optical communications modulators for next-generation computing systems.

While work in academia suggests that conducting oxides can enable a new class of plasmonic devices, the demonstrated technology remains extremely immature. Our work examined potential limitations of these unconventional materials to determine the impact on device performance.



## Quantitative Temperature Measurement of Electrically-Driven Bridge for Model Validation

192703 | Year 1 of 1 | Principal Investigator: D. Farrow

### Project Purpose:

Several key nuclear weapon (NW) components rely on electrically driven, thermally initiated plasma generation. For example, exploding bridgewire initiators (EBWs) provide a shock impulse to an explosive pressing when electrically driven to burst/plasma formation over the course of a few hundred nanoseconds. However, reliance on traditional rules of thumb for bridge design has not provided sufficient performance margin given the current LEP (life extension program) requirements. Exploding bridge wire performance has been difficult to predict for some of EBW-initiated components, based solely on previous designs. Trouble shooting unexpected challenges has added significant cost to the design process. In many cases, improper function of the bridge led to weak shock delivery into the explosive pressing. There is an urgent need to better evaluate and optimize bridge wire parameters given the unique materials sets and requirements for each detonator.

We have demonstrated emissivity compensated pyrometry (ECP) with microsecond detection to quantitatively measure temperature evolution of bridge materials electrically driven to break down. Traditional two-color pyrometry requires emissivity be wavelength independent at the probe wavelengths or that wavelength-dependent variations are known to quantitatively recover temperature. However, these assumptions break down in bridge/electrode materials driven to breakdown where temperature (300-20,000K), phase, and volume change on nanosecond time scales may cause unpredictable shifts in band structure and, therefore, the wavelength-dependent emissivity over the course of the experiment. ECP measures both reflectivity and emission simultaneously to determine both emissivity and temperature at each point using the relationship:  $\text{emissivity}(l, Q) = 1 - R(l, Q)$  (Bertness 2000). The goal of the project was to demonstrate this technique with improved time resolution to enable the first reliable, time-resolved measurements of the bridge surface during function required for equation of state (EOS) validation.

## Statistically Rigorous Uncertainty Quantification for Physical Parameter Model Calibration with Functional Output

195307 | Year 1 of 1 | Principal Investigator: L. Hund

### Project Purpose:

The S&T question inspiring this research was: how should Bayesian model calibration (BMC) with functional output be applied to estimate physical parameters in the presence of multiple sources of uncertainty, including model misspecification? The model calibration literature primarily focuses on calibration for the purpose of predicting from the model, rather than calibration for estimating underlying physical parameters that are model inputs. The research was motivated by the need to solve an inverse problem to estimate dynamic material properties from experiments conducted on the Z machine at Sandia. The limited existing work in this area uses fully Bayesian statistical model with estimation of a discrepancy function using Gaussian processes, which are computationally instable and inherently nonidentifiable, resulting in potential underestimation of uncertainty in parameter estimates.

To address the S&T question, we investigated methods for simplifying and adding robustness to the best practice full BMC framework. We introduced the notion of scaling the likelihood function by an effective sample size to adjust for autocorrelation in the functional output, as well as the concept of modularization of nuisance parameter uncertainties within the Bayesian model calibration procedure to mitigate underestimation of uncertainty in the presence of model misspecification.



## Stress-Induced Block Copolymer Lithography

191078 | Year 1 of 1 | Principal Investigator: C. Ting

### Project Purpose:

Block copolymers (BCP), two chemically incompatible polymers joined together, can self-assemble into a variety of nanostructures on length scales below 10 nm, making them ideal building blocks in applications such as nanolithography and nanotemplating. Although these nanostructures overcome the resolution of conventional top-down lithography, several challenges remain. In particular, precise, long-range order is required, whereas the spontaneous self-assembly of BCPs includes defects and randomly oriented ordered regions, separated by grain boundaries. While directed BCP self-assembly has demonstrated initial successes, these prior techniques are limited by complex pre-patterning steps, followed by time-consuming (hours to days) temperature or solvent annealing methods.

Fan et al. have recently demonstrated a facile and efficient pressure-based approach to fabricate ordered, dense, macroscopic arrays of gold nanoparticles. The method is not restricted by the resolution limitations of conventional photolithography, nor the serial (prohibitively slow) throughput of electron beam lithography (EBL) and scanning probe lithography (SPL) techniques. Motivated by the extension of this technique to "direct" the assembly BCP nanostructures, we develop a foundation for a theoretical understanding of the pressure effects on BCPs.

Because the effects of pressure on the thermodynamics and kinetics of BCP nanostructures are unexplored, developing a predictive model to provide new theoretical understanding will be a key component guiding future fundamental demonstrations of pressure-induced BCP self-assembly. In this project, we have chosen to focus on the local stress profiles of interfaces, which are essential to the phase behavior and the preferred nanostructures formed by the BCPs. From these local stress profiles, one can develop a microscopic understanding for the molecular dependence of macroscopic elastic properties, such as lateral surface tension and spontaneous curvature, which forms the foundation for a theoretically-informed pressure based self-assembly technique for BCP nanostructures.

## System Level Design of Jointed Interfaces via Advanced Manufacturing Techniques

198371 | Year 1 of 1 | Principal Investigator: M. R. Brake

### Project Purpose:

If a strategy existed for using additive manufacturing (AM) to design systems instead of parts, then the uncertainty associated with the loads being transmitted across interfaces could be reduced, improving our ability to design for specific environments. Structural engineers are good at predicting the vibrations and structural dynamics of single parts (i.e., monolithic specimens). However, once these parts are assembled into larger systems, there are no accurate models to predict the dynamics due to the interfaces between two or more joined parts. Further complicating matters, high variability/nonrepeatability is observed in experiments of the same structure due to physical processes in the joint that are not well understood (25% variation in stiffness, 300% variation in damping for some typical applications, with predictions of energy dissipation often off by orders of magnitude). With the recent investment in AM and topology optimization, parts are fabricated that have optimal behavior on their own with no regard for their behavior in an assembly.

Thus, the central question of this research is: how can interfaces be incorporated into a design while maintaining the ability to predict the system's dynamics? Two separate approaches are studied: 1) the redesign of the interface geometry and 2) the redesign of the support structure. The redesign of the interface geometry is inspired by applying theories developed within the solid mechanics communities to structural dynamics problems. The redesign of the far-field structure surrounding the joint is motivated by recent research that shows it is possible to design a nonlinear vibration absorber to cancel out the effects of a nonlinearity within a system. Several different candidate systems were designed and tested. This research differed from previous work in several ways: 1) the dynamic properties of AM parts were characterized for the first time, 2) new hypotheses for linearizing an interface were tested, and 3) a new nonlinear vibration absorption theory was experimentally tested.





## The Green Machine: Light Starved Communication beyond the Classical Limit

195305 | Year 1 of 1 | Principal Investigator: T. S. Luk

### Project Purpose:

Many of Sandia's nuclear and national security missions require extracting the maximum amount of data in photon-starved environments—including in space, underwater, at night, and through opaque materials. For example, the Mars Reconnaissance Orbiter (MRO) has sent over 50 terabytes of data to Earth using radio frequency transmitters, but even at its top data rate of 5.2 Mbps, it still takes MRO over an hour to send a single high resolution image. This project will address this optical communication problem in light-starved conditions.

Our goal to demonstrate a quantum superadditivity approach, which can increase the data rate of an optical communications system from a classical limit of 1.8 bits per photon to near 3 bits per photon in light-starved conditions, resulting in much more data with the same amount of light. Quantum superadditivity is accomplished by a remarkable collection of passive optical components arranged in such a way to either split a photon into multiple phase-coherent channels, or funnel multiple phase-coherent channels into a single output channel. This black box is called green machine (GM). A 3-bit word can be encoded in a set of 8 phases. Decoding these phases correctly would result in a photon count in the correct channel and thus 3 bits of information received from single-photon detection.

## Tritium-Based Accelerated Aging

198368 | Year 1 of 1 | Principal Investigator: B. R. Muntifering

### Project Purpose:

Helium enters material through a number of mechanisms, including tritium decay. Due to its insolubility in most materials, helium tends to form high pressure nanoscale bubbles which have a detrimental impact on mechanical properties and can cause materials to become prone to unpredictable fracture and catastrophic release of helium. Systematic experimental studies of helium evolution resulting from tritium decay are extremely time consuming, expensive, and difficult due to the 12.3-year half-life of tritium and the complexity of radiological transmission electron microscope (TEM) sample preparation. The lack of realistic, validated accelerated aging methods has slowed progress in understanding helium bubble evolution.

Sandia's in situ ion irradiation transmission electron microscopy (TEM) ( $I^3$ TEM) can be used to directly implant helium ions, at energies ranging from 100s of eV to 10s of keV, into TEM films. This allows the observation of helium bubble nucleation, growth, and coalescence in real time with nanometer resolution. The bubble lifecycle can be compressed from decades to hours and eliminates radiological concerns.

For accelerated aging studies that involve direct helium implantation, it is critical that implanted helium ions have similar energies to the helium introduction method of real world components since the defect environment induced by the helium is dependent on the helium energy, and will directly affect the bubble evolution. Tritium decay produces low energy helium, which does not produce additional lattice defects. It is not known if low energy helium (100s of eV), which is below the knock-on damage level in most metals, can be employed to successfully mimic tritium decay.

This study involved the optimization of recent modifications made to helium ion accelerator and associated beam line which allowed for in situ helium implantation into TEM samples at energies below knock-on damage levels. To test the feasibility of such a setup, gold foils were implanted with approximately 430 eV helium ions and the associated microstructural features were characterized with TEM.



## Understanding Velocity of Detonation in Graded Density Energetic Materials

195304 | Year 1 of 1 | Principal Investigator: J. C. Rodriguez

### Project Purpose:

In this project, we attempt to address a lack in our science-based understanding of the relationship between graded density materials and velocity of detonation (VoD), a density and configuration dependent explosive property that is a measure of how quickly a detonation wave propagates through an explosive sample. VoD is typically measured using time of arrival detection (TOAD) pins or break wires to measure the transient time of an explosive shock over a known distance. These measurements provide an average VoD over the sample length. Unfortunately, time of arrival techniques are hard to implement at small length scales and limit data collection to a number of discrete data points.

This study will investigate VoD with graded densities of energetic material. Energetic materials with graded densities may exhibit different timing characteristics while still achieving the same output performance. These materials will help us better understand the relationship between material properties, VoD, and output performance. These studies will help us understand and then predict the performance of existing and new energetic material compositions in the stockpile



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## Unpublished Summaries

For information on the following FY 2016 LDRD Projects, please contact the LDRD Office:

Laboratory Directed Research and Development  
Sandia National Laboratories  
Albuquerque, NM 87185-0359

### Project Title

- 173115 Advanced Deprocessing Techniques to Investigate White Light LVP and other Imaging
- 173128 Seebeck Enhancement via Quantum Confinement in MOSFET's: Towards Monolithic On-Chip Cooling
- 180827 Additive Manufacturing of Integrated Functional Materials
- 180829 Mitigating Information Disclosure Vulnerabilities
- 180842 Biologically-Enabled Remote Sensing for Real-Time Detection and Threat Response
- 180844 Pulsed Ultraviolet Light-Assisted Chemical Etching for F/A of Advanced CMOS Circuitry
- 180848 Electromagnetic Propagation and Prediction
- 180850 Using Graphene to Enable Trusted Microelectronics
- 180852 An Ultra-low SWaP Multi-Mission Bi-Static Sensor
- 180891 Emulation for Cyber-Enabled Physical Attack Scenarios
- 180930 Microenergetic Logic for Safety Applications
- 190971 Green Monopropellant System Design and Characterization for Threat Signature Analyses
- 190974 Optical Technology
- 190975 Novel Applications of the Multi-Beam SEM
- 190989 Creating Data for Validating Machine Learning Methods
- 190994 Shot Noise Limited Imaging with Lock-In Based Focal Plane Arrays
- 190998 Microscale Transient Detection
- 191000 Advanced Materials and Devices for Communications
- 191002 Tunable Inkjet Materials
- 191005 Development and Demonstration of Alternative Precision Navigation Capabilities in GPS-Denied Environments
- 191006 Understanding Photon / Free Carrier Interaction in Low Vapor Pressure Signals on Ultra-Thin Silicon Integrated Circuits
- 191014 Stress-Induced Emission
- 191080 Phononic Manipulation of the Superconducting State
- 191129 Digital Rock Physics for Multi-Scale Experiments and Modeling of Fractured Porous Media
- 191152 Airborne Defense Against the Small Unmanned Aircraft Systems (UAS) Threat
- 191239 Adjoint-Based Methods for Optimization and Uncertainty Quantification in Particle Transport
- 192870 Synthetic Aperture Radar Targeting for Prompt Global Strike Missions
- 196225 Piezoelectric-Magnetostrictive Transceiver Concept
- 198369 'Tattle-tale,' Ion-Implanted Nanoparticle, Strengthened Steels



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## Awards and Recognition

PI	Award	Project
Hope Michelsen	Invited contributors, 2016 Greenhouse Gas & Emissions Reporting & Analysis System, DOE Big Idea, Big Idea Summit.	173100
Patrick Griffin	NNSA Defense Programs Award of Excellence	173104
Christine Coverdale	IEEE Plasma Science and Applications Award	173104
	Prism Award, Society of Women Engineers	173104
Mark Savage	William Dunbar Award, IEEE	173104
Robert Kolasinski	Early Career Award, Department of Energy	173104
Marissa Anderson Conroy	Outstanding Graduate Student/Technologist Poster Award, 27th Rio Grande Symposium on Advanced Materials	173110
Samantha Lawrence	TMS Young Leader Award	173116
Jon Ihlefeld	Best Poster Award, 2016 Materials Research Society Spring Meeting	173117
	Ferroelectrics Young Investigator Award, IEEE Ultrasonics Ferroelectrics and Frequency Control Society	173117
Mark Musculus	Fellow, SAE International	173664
Cynthia Phillips	Distinguished Scientist, Association of Computing Machinery	180820
	Best Paper Award, 14th USENIX Conference on File and Storage Technologies	180820
	Fellow, Society for Industrial and Applied Mathematics	180820
Julie Parish	Outstanding Young Aerospace Engineer, Texas A&M University, Aerospace Engineering Department.	180826
Mark Rodriguez	Elected as Technical Committee Chairman for the International Centre for Diffraction Data (ICDD)	180857
Justin Wagner	Best AMT Paper, 2016 AIAA Aerospace Sciences Meeting.	180876
Conrad James	R&D100 Award Finalist in the IT/Electrical, Software/Services, and Special Recognition: Market Disruptor categories	180885
	Black Engineer of the Year Award, Professional achievement category.	180885
Catherine Sobczak	Thin Film Division Distinguished Technologist Award, American Vacuum Society	180926
Bernadette Hernandez- Sanchez	Hispanic Engineer National Achievement Awards Conference award	190245
Jeff Brinker	Elected to the National Academy of Inventors	190960
Laura Matzen, Laura McNamara	Federal Laboratory Consortium Mid-Continent Region, Notable Technology Award, for GazeAppraise	190967
Joshua Beutler	Best Paper Award, 2015 International Symposium	191006
Ali Pinar	Distinguished Scientist, Association of Computing Machinery	191009
Phillip Reu	Brewer Award, Outstanding Experimentalist, Society of Experimental Mechanics	191068
Vince Urias	Best Paper Award, 2016 IEEE International Symposium on Technologies for Homeland Security	191165
	Hispanic Engineer National Achievement Awards Conference award	191165
Jon Ihlefeld	IEEE-UFFC Ferroelectrics Young Investigator Award	191197



PI	Award	Project
Timothy Lambert	Best Paper Award, 2016 AIChE Rocky Mountain Student Regional Conference Meeting.	195216
	Best Paper Award, 2016 Society of Women Engineers Region ABJ 2016 Conference.	195216
Hongyou Fan	Fellow, Materials Research Society	173121
David Osborn	Fellow, American Physical Society	176312
John Porter	R&D 100 Award & R&D 100 Market Disruptor Product Special Recognition Award, Ultra-fast X-ray Imager	130805
Ryan Camacho	R&D 100 Award, Transceiver for Quantum Keys & Encryption	173103
William Hart	R&D 100 Award, Pyomo v4.1	130742
Hongyou Fan	R&D 100 Award, Stress-Induced Fabrication of Functionally Designed Nanomaterials	155412
Summer Ferreira	R&D 100 Green Tech Special Recognition Award, Precion High Power Battery Tester	166152



## Publications

The following peer-reviewed publications, published in 2015, are attributed to the LDRD projects noted in the table below. Because publications are tallied over the calendar year, and Sandia operates on a fiscal year, publication metrics for 2016 will be reported in the 2017 Annual Report.

Authors	Article Title	Source	Vol.	No.	Pg.	Project
Ibtesham, Dewan; Ferreira, Kurt B.; Arnold, Dorian	A checkpoint compression study for high-performance computing systems	INTERNATIONAL JOURNAL OF HIGH PERFORMANCE COMPUTING APPLICATIONS	29	4	387-402	158802
Drewry, J. L.; Choi, C. Y.; An, L.; Gharagozloo, P. E.	A computational fluid dynamics model of algal growth: development and validation	TRANSACTIONS OF THE ASABE	58	2	203-213	153236
Wojciechowski, Kenneth E.; Baker, Michael S.; Clews, Peggy J.; Olsson, Roy H., III	A Fully Integrated Oven Controlled Microelectromechanical Oscillator-Part I: Design and Fabrication	JOURNAL OF ELECTROMECHANICAL SYSTEMS	24	6	1782-1794	173048
Tu-Thach Quach; Malinas, Rebecca; Koch, Mark W.	A Model-Based Approach to Finding Tracks in SAR CCD Images	2015 IEEE CONFERENCE ON COMPUTER VISION AND PATTERN RECOGNITION WORKSHOPS (CVPRW)	--	--	41-47	165535
Lehoucq, R. B.; Reu, P. L.; Turner, D. Z.	A Novel Class of Strain Measures for Digital Image Correlation	STRAIN	51	4	265-275	188029
Mitchell, John A.; Silling, Stewart A.; Littlewood, David J.	A position-aware linear solid constitutive model for peridynamics	JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES	10	5	539-557	165616
Chaudhry, Jehanzeb H.; Estep, Donald; Ginting, Victor; Shadid, John N.; Tavener, Simon	A posteriori error analysis of IMEX multi- step time integration methods for advection- diffusion-reaction equations	COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING	285		730-751	173026
Williams, Jeffery T.; Bacon, Larry D.; Walker, Michael J.; Zeek, Erik C.	A Robust Approach for the Analysis of EMI/EMC Problems With Nonlinear Circuit Loads	IEEE TRANSACTIONS ON ELECTROMAGNETIC COMPATIBILITY	57	4	680-687	158773
Leenheer, Andrew J.; Sullivan, John P.; Shaw, Michael J.; Harris, C. Thomas	A Sealed Liquid Cell for In Situ Transmission Electron Microscopy of Controlled Electrochemical Processes	JOURNAL OF ELECTROMECHANICAL SYSTEMS	24	4	1061-1068	158810
Cox, Jonathan A.; James, Conrad D.; Aimone, James B.	A Signal Processing Approach for Cyber Data Classification with Deep Neural Networks	COMPLEX ADAPTIVE SYSTEMS, 2015	61	--	349-354	180885
Jebail, Mais J.; Renzi, Ronald F.; Sinha, Anupama; Van De Vreugde, Jim; Gondhalekar, Carmen	A solvent replenishment solution for managing evaporation of biochemical reactions in air-matrix digital microfluidics devices	LAB ON A CHIP	15	1	151-158	158814
Jha, Madhav; Seshadhri, C.; Pinar, Ali	A Space-Efficient Streaming Algorithm for Estimating Transitivity and Triangle Counts Using the Birthday Paradox	ACM TRANSACTIONS ON KNOWLEDGE DISCOVERY FROM DATA	9	3	--	158477



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Ampleford, David J.; Bland, Simon N.; Jennings, Christopher A.; Lebedev, Sergey V.; Chittenden, Jeremy P.	Investigating Radial Wire Array Z-Pinches as a Compact X-Ray Source on the Saturn Generator	IEEE TRANSACTIONS ON PLASMA SCIENCE	43	9	3344-3352	117862
Beechem, Thomas; Yates, Luke; Graham, Samuel	Invited Review Article: Error and uncertainty in Raman thermal conductivity measurements	REVIEW OF SCIENTIFIC INSTRUMENTS	86	4	--	173124
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Crawford, Mary H.; Allerman, Andrew A.; Armstrong, Andrew M.; Smith, Michael L.; Cross, Karen C.	Laser diodes with 353nm wavelength enabled by reduced- dislocation-density AlGaIn templates	APPLIED PHYSICS EXPRESS	8	11	--	158857
Harper, Jason C.; Carson, Bryan D.; Bachand, George D.; Arndt, William D.; Finley, Melissa R.	Laser Machined Plastic Laminates: Towards Portable Diagnostic Devices for Use in Low Resource Environments	ELECTROANALYSIS	27	11	2503-2512	158813
Michelsen, H. A.; Schulz, C.; Smallwood, G. J.; Will, S.	Laser-induced incandescence: Particulate diagnostics for combustion, atmospheric, and industrial applications	PROGRESS IN ENERGY AND COMBUSTION SCIENCE	51	--	02-48	173094
Schollmeier, M.; Sefkow, A. B.; Geissel, M.; Arefiev, A. V.; Flippo, K. A.	Laser-to-hot-electron conversion limitations in relativistic laser matter interactions due to multi-picosecond dynamics	PHYSICS OF PLASMAS	22	4	--	151367



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Wu, Re-Bing; Brif, Constantin; James, Matthew R.; Rabitz, Herschel	Limits of optimal control yields achievable with quantum controllers	PHYSICAL REVIEW A	91	4	--	173103
Scheer, Adam M.; Welz, Oliver; Vasu, Subith S.; Osborn, David L.; Taatjes, Craig A.	Low temperature (550-700 K) oxidation pathways of cyclic ketones: dominance of HO <sub>2</sub> -elimination channels yielding conjugated cyclic coproducts	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	17	18	12124-12134	151308
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Harrison, Katharine L.; Biedermann, Laura B.; Zavadil, Kevin R.	Mechanical Properties Langmuir Monolayers: Article of Water-Assembled Graphene Oxide Guiding Controlled Transfer	LANGMUIR	31	36	9825-9832	158183
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Pirrone, Gregory F.; Emert-Sedlak, Lori A.; Wales, Thomas E.; Smithgall, Thomas E.; Kent, Michael S.	Membrane-Associated Conformation of HIV-1 Nef Investigated with Hydrogen Exchange Mass Spectrometry at a Langmuir Monolayer	ANALYTICAL CHEMISTRY	87	14	7030-7035	158832
Sridharan, Vilas; DeBardeleben, Nathan; Blanchard, Sean; Ferreira, Kurt B.; Stearley, Jon	Memory Errors in Modern Systems	ACM SIGPLAN NOTICES	50	4	297-310	158802
Wu, Meiye; Singh, Anup K.	Microfluidic Flow Cytometry for Single-Cell Protein Analysis	SINGLE CELL PROTEIN ANALYSIS: METHODS AND PROTOCOLS	1346	--	69-83	95215
Burckel, D. Bruce; Resnick, Paul J.; Finnegan, Patrick S.; Sinclair, Michael B.; Davids, Paul S.	Micrometer-scale fabrication of complex three dimensional lattice plus basis structures in silicon	OPTICAL MATERIALS EXPRESS	5	10	2231-2239	173129
Castelluccio, Gustavo M.; McDowell, David L.	Microstructure and mesh sensitivities of mesoscale surrogate driving force measures for transgranular fatigue cracks in polycrystals	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	639	--	626-639	193072



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Black, Dolores A.; Robinson, William H.; Wilcox, Ian Z.; Limbrick, Daniel B.; Black, Jeffrey D.	Modeling of Single Event Transients With Dual Double-Exponential Current Sources: Implications for Logic Cell Characterization	IEEE TRANSACTIONS ON NUCLEAR SCIENCE	62	4	1540-1549	181198
Rogers, David M.; Kent, Michael S.; Rempe, Susan B.	Molecular basis of endosomal-membrane association for the dengue virus envelope protein	BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES	1848	4	1041-1052	158832
Wood, M. R.; Kanedy, K.; Lopez, F.; Weimer, M.; Klem, J. F.	Monolayer-by-monolayer compositional analysis of InAs/InAsSb superlattices with cross-sectional STM	JOURNAL OF CRYSTAL GROWTH	425		110-114	165717
Kuhlman, Kristopher L.; Malama, Bwalya; Heath, Jason E.	Multiporosity flow in fractured low-permeability rocks	WATER RESOURCES RESEARCH	51	2	848-860	165670
Gamble, John King; Jacobson, N. Tobias; Nielsen, Erik; Baczewski, Andrew D.; Moussa, Jonathan E.	Multivalley effective mass theory simulation of donors in silicon	PHYSICAL REVIEW B	91	23 518	--	173883
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Wang, Xueju; Pan, Zhipeng; Fan, Feifei; Wang, Jiangwei; Liu, Yang	Nanoscale Deformation Analysis With High-Resolution Transmission Electron Microscopy and Digital Image Correlation	JOURNAL OF APPLIED MECHANICS-TRANSACTIONS OF THE ASME	82	12		158810
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Mason, P. E.; Ansell, S.; Neilson, G. W.; Rempe, S. B.	Neutron Scattering Studies of the Hydration Structure of Li <sup>+</sup>	JOURNAL OF PHYSICAL CHEMISTRY B	119	5	2003-2009	165696
Mengesha, Wondwosen; Kiff, Scott D.	Neutron Spectrometry for UF <sub>6</sub> Enrichment Verification in Storage Cylinders	IEEE TRANSACTIONS ON NUCLEAR SCIENCE	62	1	272-280	151315
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Li, Changyi; Wright, Jeremy B.; Liu, Sheng; Lu, Ping; Figiel, Jeffrey J.	Nonpolar InGa <sub>N</sub> /Ga <sub>N</sub> multi-quantum-well core-shell nanowire lasers	2015 CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO)	--	--	--	165704
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Thoma, C.; Genoni, T. C.; Welch, D. R.; Rose, D. V.; Clark, R. E.	Numerical simulation of cathode plasma dynamics in magnetically insulated vacuum transmission lines	PHYSICS OF PLASMAS	22	3	--	173104
Lu, Ping; Yan, Pengfei; Romero, Eric; Spoerke, Erik David; Zhang, Ji-Guang	Observation of Electron-Beam-Induced Phase Evolution Mimicking the Effect of the Charge-Discharge Cycle in Li-Rich Layered Cathode Materials Used for Li Ion Batteries	CHEMISTRY OF MATERIALS	27	4	1375-1380	180899
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Argibay, N.; Mogonye, J. E.; Michael, J. R.; Goeke, R. S.; Kotula, P. G.	On the thermal stability of physical vapor deposited oxide-hardened nanocrystalline gold thin films	JOURNAL OF APPLIED PHYSICS	117	14	--	158856
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Harper-Slaboszewicz, Victor J.; Leckbee, Joshua; Bennett, Nichelle; Madrid, Elizabeth A.; Rose, David V.	Parallel Operation of Multiple Closely Spaced Small Aspect Ratio Rod Pinches	IEEE TRANSACTIONS ON PLASMA SCIENCE	43	1	422-432	165738
Frank, Joel C.; Frank, Shayna M.; Thurlow, Lincoln A.; Kroeger, Thomas M.; Miller, Ethan L.	Percival: A Searchable Secret-Split Datastore	2015 31ST SYMPOSIUM ON MASS STORAGE SYSTEMS AND TECHNOLOGIES (MSST)	--	--	--	180820
King, M. P.; Armstrong, A. M.; Dickerson, J. R.; Vizkelethy, G.; Fleming, R. M.	Performance and Breakdown Characteristics of Irradiated Vertical Power GaN P-i-N Diodes	IEEE TRANSACTIONS ON NUCLEAR SCIENCE	62	6	2912-2918	180884
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Xiao, Xiaoyin; Fischer, Arthur J.; Coltrin, Michael E.; Lu, Ping; Koleske, Daniel D.	Photoelectrochemical etching of epitaxial InGa <sub>N</sub> thin films: self-limited kinetics and nanostructuring	ELECTROCHIMICA ACTA	162	--	163-168	191196
Gies, Christopher; Jahnke, Frank; Chow, Weng W.	Photon antibunching from few quantum dots in a cavity	PHYSICAL REVIEW A	91	6	--	173103
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Hooper, R. J.; Davis, C. G.; Johns, P. M.; Adams, D. P.; Hirschfeld, D.	Prediction and characterization of heat-affected zone formation in tin-bismuth alloys due to nickel-aluminum multilayer foil reaction	JOURNAL OF APPLIED PHYSICS	117	24	--	173653
Silling, Stewart; Weckner, Olaf	Preface	JOURNAL OF MECHANICS OF MATERIALS AND STRUCTURES	10	5	537-537	165616
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Reisman, D. B.; Stoltzfus, B. S.; Stygar, W. A.; Austin, K. N.; Waisman, E. M.	Pulsed power accelerator for material physics experiments	PHYSICAL REVIEW SPECIAL TOPICS-ACCELERATORS AND BEAMS	18	9	--	173191
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Gong, Ke; Martin, James E.; Shea-Rohwer, Lauren E.; Lu, Ping; Kelley, David F.	Radiative Lifetimes of Zincblende CdSe/CdS Quantum Dots	JOURNAL OF PHYSICAL CHEMISTRY C	119	4	2231-2238	165697



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Rogge, Paul C.; Thuermer, Konrad; Foster, Michael E.; McCarty, Kevin F.; Dubon, Oscar D.	Real-time observation of epitaxial graphene domain reorientation	NATURE COMMUNICATIONS	6	6850	--	165698
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Vineyard, Craig M.; Verzi, Stephen J.; James, Conrad D.; Aimone, James B.; Heileman, Gregory L.	Repeated Play of the SVM Game as a Means of Adaptive Classification	2015 INTERNATIONAL JOINT CONFERENCE ON NEURAL NETWORKS (IJCNN)	--	--	--	180885
Koch, Mark W.; Moya, Mary M.; Chow, Jim G.; Goold, Jeremy; Malinas, Rebecca	Road Segmentation using Multipass Single-Pol Synthetic Aperture Radar Imagery	2015 IEEE CONFERENCE ON COMPUTER VISION AND PATTERN RECOGNITION WORKSHOPS (CVPRW)	--	--	--	165535
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Riviello, Gregory; Tibbetts, Katharine Moore; Brif, Constantin; Long, Ruixing; Wu, Re-Bing	Searching for quantum optimal controls under severe constraints	PHYSICAL REVIEW A	91	4	--	154059
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Romero, Natalia; Nozick, Linda K.; Dobson, Ian; Xu, Ningxiong; Jones, Dean A.	Seismic Retrofit for Electric Power Systems	EARTHQUAKE SPECTRA	31	2	1157-1176	151313
Wierer, Jonathan J., Jr.; Allerman, Andrew A.; Skogen, Erik J.; Tauke-Pedretti, Anna; Vawter, Gregory A.	Selective layer disordering in intersubband Al <sub>0.028</sub> Ga <sub>0.972</sub> N/AlN superlattices with silicon nitride capping layer	APPLIED PHYSICS EXPRESS	8	6	--	158830



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Lou, Yan-Ru; Kanninen, Liisa; Kaehr, Bryan; Townson, Jason L.; Niklander, Johanna	Silica bioreplication preserves three-dimensional spheroid structures of human pluripotent stem cells and HepG2 cells	SCIENTIFIC REPORTS	5	--	--	190960
VanDelinder, Virginia; Wheeler, David R.; Small, Leo J.; Brumbach, Michael T.; Spoerke, Erik D.	Simple, Benign, Aqueous-Based Amination of Polycarbonate Surfaces	ACS APPLIED MATERIALS & INTERFACES	7	10	5643-5649	165696
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Johnston, Robert; Rogelj, Snezna; Harper, Jason C.; Tartis, Michaelann	Sol-Generating Chemical Vapor into Liquid (SG-CViL) deposition - a facile method for encapsulation of diverse cell types in silica matrices	JOURNAL OF MATERIALS CHEMISTRY B	3	6	1032-1041	190960
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Ihlefeld, Jon F.; Kotula, Paul G.; Gauntt, Bryan D.; Gough, Dara V.; Brennecke, Geoff L.	Solution Chemistry, Substrate, and Processing Effects on Chemical Homogeneity in Lead Zirconate Titanate Thin Films	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	98	7	2028-2038	159257
Thompson, A. P.; Swiler, L. P.; Trott, C. R.; Foiles, S. M.; Tucker, G. J.	Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials	JOURNAL OF COMPUTATIONAL PHYSICS	285	--	316-330	158794
Abdeljawad, Fadi; Foiles, Stephen M.	Stabilization of nanocrystalline alloys via grain boundary segregation: A diffuse interface model	ACTA MATERIALIA	101	--	159-171	191240
Zhang, Wenrui; Chen, Aiping; Jian, Jie; Zhu, Yuanyuan; Chen, Li	Strong perpendicular exchange bias in epitaxial La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub> :BiFeO <sub>3</sub> nanocomposite films through vertical interfacial coupling	NANOSCALE	7	33	13808-13815	180899
Yang, Sang Mo; Lee, Shinbuhm; Jian, Jie; Zhang, Wenrui; Lu, Ping	Strongly enhanced oxygen ion transport through samarium-doped CeO <sub>2</sub> nanopillars in nanocomposite films	NATURE COMMUNICATIONS	6	--	--	180923
Boyle, Timothy J.; Sears, Jeremiah M.; Neville, Michael L.; Alam, Todd M.; Young, Victor G., Jr.	Structural Properties of the Acidification Products of Scandium Hydroxy Chloride Hydrate	INORGANIC CHEMISTRY	54	24	11831-11841	173156
Ting, Christina L.; Stevens, Mark J.; Frischknecht, Amalie L.	Structure and Dynamics of Coarse-Grained Ionomer Melts in an External Electric Field	MACROMOLECULES	48	3	809-818	165824



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Campione, Salvatore; Basilio, Lorena I.; Warne, Larry K.; Sinclair, Michael B.	Tailoring dielectric resonator geometries for directional scattering and Huygens' metasurfaces	OPTICS EXPRESS	23	3	2293-2307	189614
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Aytac, Y.; Olson, B. V.; Kim, J. K.; Shaner, E. A.; Hawkins, S. D.	Temperature dependent carrier lifetime measurements of InAs/InAsSb T2SLs	QUANTUM SENSING AND NANOPHOTONIC DEVICES XII	9370	--	--	165703
Aytac, Y.; Olson, B. V.; Kim, J. K.; Shaner, E. A.; Hawkins, S. D.	Temperature-dependent optical measurements of the dominant recombination mechanisms in InAs/InAsSb type-2 superlattices	JOURNAL OF APPLIED PHYSICS	118	12	--	165703
Mitrofanov, O.; Yu, W.; Thompson, R. J.; Jiang, Y.; Greenberg, Z. J.	Terahertz near-field imaging of surface plasmon waves in graphene structures	SOLID STATE COMMUNICATIONS	224	--	47-52	158829
Biedermann, G. W.; Wu, X.; Deslauriers, L.; Roy, S.; Mahadeswaraswamy, C.	Testing gravity with cold-atom interferometers	PHYSICAL REVIEW A	91	3	--	173130
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Bartsch, Michael S.; Edwards, Harrison S.; Lee, Daniel; Moseley, Caroline E.; Tew, Karen E.	The Rotary Zone Thermal Cycler: A Low-Power System Enabling Automated Rapid PCR	PLOS ONE	10	3	--	158814
Hudson, Corey M.; Williams, Kelly P.	The tmRNA website	NUCLEIC ACIDS RESEARCH	43	D1	DD38-D140	165683
Cheaito, Ramez; Gorham, Caroline S.; Misra, Amit; Hattar, Khalid; Hopkins, Patrick E.	Thermal conductivity measurements via time-domain thermoreflectance for the characterization of radiation induced damage	JOURNAL OF MATERIALS RESEARCH	30	9	1403-1412	165741
Alaie, Seyedhamidreza; Goettler, Drew F.; Su, Mehmet; Leseman, Zayd C.; Reinke, Charles M.	Thermal transport in phononic crystals and the observation of coherent phonon scattering at room temperature	NATURE COMMUNICATIONS	6	7228	--	173128
Lee, Jonathan W.; Meade, Andrew J., Jr.; Barrera, Enrique V.; Templeton, Jeremy A.	Thermal Transport Mechanisms in Carbon Nanotube-Nanofluids Identified From Molecular Dynamics Simulations	JOURNAL OF HEAT TRANSFER-TRANSACTIONS OF THE ASME	137	7	--	151294
Erickson, Kristopher J.; Leonard, Francois; Stavila, Vitalie; Foster, Michael E.; Spataru, Catalin D.	Thin Film Thermoelectric Metal-Organic Framework with High Seebeck Coefficient and Low Thermal Conductivity	ADVANCED MATERIALS	27	22	3453-3459	180898
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Cui, Yu Yan; Brioude, Jerome; McKeen, Stuart A.; Angevine, Wayne M.; Kim, Si-Wan	Top-down estimate of methane emissions in California using a mesoscale inverse modeling technique: The South Coast Air Basin	JOURNAL OF GEOPHYSICAL RESEARCH-ATMOSPHERES	120	13	6698-6711	173100
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McGrew, Genette I.; Khatri, Pathik A.; Geiger, William E.; Kemp, Richard A.; Waterman, Rory	Unexpected formal insertion of CO <sub>2</sub> into the C-Si bonds of a zinc compound	CHEMICAL COMMUNICATIONS	51	87	15804-15807	151300
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## ABSTRACT

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2016. In addition to the programmatic overview, the report includes progress reports from 366 individual R&D projects in 14 categories.

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